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 H₂O₂/NaOCl) and from radiofrequency 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

¹Figures 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, O₂ [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 ${}^{3}\Sigma_{\mu}^{-}$. 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 $^3\Sigma_{\rm g}^-$ ground state. The electronic transitions $^1\Delta_{\rm g} \leftarrow ^3\Sigma_{\rm g}^-$ 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 $O_2^*(^{L}\Sigma_g^{+})$ 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 ${}^{1}\Delta_{\rho}$ 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.

$$I ext{S} + hv \rightarrow {}^{1}S^{*} \rightarrow {}^{3}S^{*}$$
; with rate $= I_{a}\Phi_{T}^{02}$

$$2 \qquad {}^{3}S^{*} + {}^{3}O_{2}({}^{3}\Sigma_{g}) \longrightarrow {}^{1}O_{2}^{*}({}^{1}\Delta_{g}) + S(k_{T\Delta})$$

$$\beta$$
 ${}^{1}\mathrm{O}_{2}^{*}({}^{1}\Delta_{g}) \longrightarrow {}^{3}\mathrm{O}_{2}({}^{3}\Sigma_{g}^{-}) (k_{d})$

4
$${}^{1}O_{2}^{*}({}^{1}\Delta_{g}) + A \rightarrow AO_{2}$$
 or other products (k_{r}^{A})

where I_a is the rate of absorption of photons by S and ϕ_T^{02} 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 ~ 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 $\sim 1~\mu s$ steps I and I above will be more than 95% complete so that, after this time, singlet oxygen decay will be given by

$$-d[{}^{1}O_{2}^{*}]/dt = (k_{d} + k_{A}[A])[{}^{1}O_{2}^{*}]$$
 (1)

and therefore

$$[^{1}O_{2}^{*}] = [^{1}O_{2}^{*}]_{t=0} [\exp{-(k_{d}t + \int_{0}^{t} k_{A}[A]dt)}].$$
 (2)

From reaction 4

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

and therefore

$$-d[A] = k_r^{A}[A][{}^{1}O_2^{*}]_{t=0}[\exp{-(k_d t + \int_0^t k_A[A]dt)}]dt$$
(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 $\sim 10\%$) and then integration of eq (4) gives, taking $k_{\rm D} = k_{\rm d} + k_{\rm A}[{\rm A}]_{\rm av}$

[A] - [A]_m =
$$(k_r^A[^1O_2^*]_{t=0}[A]_{av}/k_D)[\exp(-k_Dt)]$$
 (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.

$$[A]_{t} - [A]_{\infty} = \Delta A/\epsilon l, \qquad (6)$$

where ϵ is the extinction coefficient and l the analyzing pathlength, 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

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

or

$$\ln ([A]/[A]_{\infty}) = (k_r^A[^1O_2^*]_{t=0}/k_D)[\exp(-k_Dt)]$$
 (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 $k_{\rm D}$ using eqs (5) or (7) and (8) give agreement to within $\pm 5\%$ and do not differ, within an experimental error of about $\pm 10\%$ 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
$${}^{1}O_{2}^{*}({}^{1}\Delta_{a}) + Q \rightarrow O_{2}({}^{3}\Sigma_{a}) + Q (k_{a}^{Q})$$

and

7
$${}^{1}O_{2}*({}^{1}\Delta_{x}) + Q \rightarrow QO_{2}$$
 or other products (k_{r}^{Q}) ,

eq (1) becomes

$$-d[{}^{1}O_{2}^{*}]/dt = (k_{d} + k_{A}[A] + k_{O}[Q])[{}^{1}O_{2}^{*}]$$
 (9)

where $k_{\rm Q}=k_{\rm r}^{\rm Q}+k_{\rm q}^{\rm Q}$ and $k_{\rm D}$ the decay constant for singlet oxygen now in the presence of a quencher becomes

$$k_{\rm D} = k_{\rm d} + k_{\rm A}[{\rm A}] + k_{\rm O}[{\rm Q}].$$
 (10)

Measurement of $k_{\rm D}$ as a function of [Q] allows values of $k_{\rm Q}$ to be obtained. N.B. If $k_{\rm Q}$ is partly due to physical quenching and partly due to reaction, the value of $k_{\rm Q}$

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
$${}^{1}O_{2}^{*}({}^{1}\Delta_{g}) + {}^{3}O_{2}({}^{3}\Sigma_{g}^{-}) \longrightarrow 2O_{2}({}^{3}\Sigma_{g}^{-}) (k_{g}^{-}),$$

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

$$k_{\rm D} = k_{\rm d} + k_{\rm A}[{\rm A}] + k_{\rm g}^{\rm O2}[{\rm O}_2].$$

However since under these conditions $k_q^{02}[O_2] > > k_d$ only values of $k_A[A]$ and k_q^{02} 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

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

$$^{1}O_{2}^{*}(^{1}\Delta_{a}) + C \rightarrow ^{3}C^{*} + ^{3}O_{2}(^{3}\Sigma_{a}^{-}) (k_{AC})$$

$$11 \qquad {}^{3}\mathrm{C}^{*} \to \mathrm{C}(k_{\mathrm{dC}})$$

12
$${}^{3}C^* + {}^{3}O_2({}^{3}\Sigma_{s}) \rightarrow \text{quenching } (k_{co})$$

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

$$[^{3}C^{*}] = (11)$$

$$U[\exp(-k_{T}t) - \exp(-k_{C}t)] + V[\exp(-k_{D}t) - \exp(-k_{C}t)]$$

where $k_{\rm T}=k_{\rm TO}[{\rm O_2}]+k_{\rm TC}[{\rm C}];~k_{\rm C}=k_{\rm CO}[{\rm O_2}]+k_{\rm dC},$ and $k_{\rm D}=k_{\rm d}+k_{\rm \Delta C}[{\rm C}]+k_{\rm Q}[{\rm Q}].$ In aerated solutions the values of $k_{\rm TO}[{\rm O_2}]$ and $k_{\rm CO}[{\rm O_2}]$ are such that after $\sim 1~\mu \rm s,~\exp(-k_{\rm c}t)$ and $\exp(-k_{\rm c}t)$ become negligibly small and eq (11) becomes

$$[^{3}C^{*}] = V \exp(-k_{D}t)$$
 (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 [O2], [C] and [Q] are constant. It is usually possible to arrange for these to be present in excess so that $[O_2] > [O_2^*]$, $[C] > [O_2^*]$ and any consumption of Q or O2 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 $k_{\rm D}$ 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 CCl₄ of 28 ms and a phosphorescence yield of 5 \times 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 CCl₄ 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.

$$\phi_0/\phi = 1 + k_0 \tau_0[Q] = 1 + [Q]/\beta_0$$
 (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_0 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.

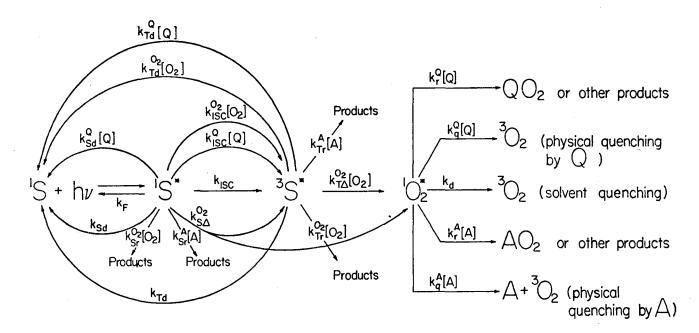


FIGURE 1. Kinetic scheme for the photosensitized formation of singlet molecular oxygen. S = sensitizer, A = oxidizable substrate, Q = physical quencher.

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 I-5 as given in section 2.1. For continuous irradiation the steady-state approximation can be applied to steps I-5 to give

Rate of oxygenation =
$$r_{ox} = I_{a} \phi_{T}^{O2} \gamma_{\Delta} k_{r}^{A} [A] / (k_{d} + k_{A} [A])$$
(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

$$r_{\rm ox}^{-1} = (I_{\rm a} \phi_{\rm T}^{02} \gamma_{\Delta} \gamma_{\rm f}^{\rm A})^{-1} \left[1 + (k_{\rm d}/k_{\rm A})(1/[{\rm A}]) \right]$$
 (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

slope/intercept =
$$k_d/k_A$$
 = β_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 $k_{\rm d}$ were reported, in which case we have taken preferred values of $k_{\rm d}$ from table 1 in order to derive values of $k_{\rm A}$ from these β values. Where authors have quoted values of $k_{\rm A}$ derived in like manner we have quoted the values of $k_{\rm d}$ they used in the comments column of the tables. When the use of preferred values for $k_{\rm d}$ gives a value of $k_{\rm A}$ 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 $\it I$ to $\it 5$ the further steps $\it 13$ and $\it 14$

13
$${}^{1}O_{2}^{*}({}^{1}\Delta_{g}) + A' \rightarrow A'O_{2}$$
 or other products $(k_{r}^{A'})$

14
$${}^{1}O_{2}*({}^{1}\Delta_{g}) + A' \rightarrow A + {}^{3}O_{2}(k_{g}^{A'})$$

(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

$$-d[A']/dt = I_a \phi_T^{02} \gamma_\Delta k_r^{A'} [A']/(k_d + k_A [A] + k_{A'} [A']),$$

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

$$-d \ln[A']/dt = I_a \phi_T^{O2} \gamma_\Delta k_r^{A'}/(k_d + k_A[A]) = S,$$

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

$$-\mathrm{d} \ln[\mathrm{A}']/\mathrm{d}t = I_{\mathrm{a}} \phi_{\mathrm{T}}^{02} \gamma_{\Delta} k_{\mathrm{r}}^{\mathrm{A}'}/k_{\mathrm{d}} = S_{0}.$$

thus

$$S_0/S = 1 + (k_A/k_d)[A] = 1 + [A]/\beta_A.$$
 (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-diphenylisobenzo-furan (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

$$(d[AO_2]/dt)/(d[A'O_2]/dt) = (17)$$

$$(-d[A]/dt)/(-d[A']/dt) = k_r^{A}[A]/k_r^{A'}[A']$$

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,

$$(r_{ox}^{0}(A)/r_{ox}^{A'}(A))_{t=0} =$$

$$1 + ([A']_{0}/\beta_{A})(1 + [A]_{0}/\beta_{A})^{-1}$$
(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

$$(r_{ox}^{Q})^{-1} =$$

$$(I_{a} \Phi_{T}^{O2} \gamma_{\Delta} \gamma_{r}^{A})^{-1} [1 + [A]^{-1} (\beta_{A} + k_{Q}[Q]/k_{A})]$$

$$(19)$$

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

slope/intercept =
$$(\beta_A + k_0[Q]/k_A)$$
 (20)

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

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

$$(slope)_0/(slope)_0 = 1 + \beta_0^{-1}[Q]$$
 (22)

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

$$(r_{ox}^{0}/r_{ox}^{Q})_{t=0} = 1 + k_{Q}[Q]/(k_{d} + k_{A}[A]_{0}) =$$

$$(23)$$

$$1 + ([Q]/\beta_{0})(1 + [A]_{0}/\beta_{A})^{-1}$$

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

$$[AO_2]_0/[AO_2] = [A]_0/\Delta[A] = A^0/\Delta A = (24)$$

$$(I_a t \Phi_T^{O_2} \gamma_\Delta \gamma_r^{\Lambda})^{-1} ([A]_0 + k_d/k_{\Lambda} + k_0[Q]/k_{\Lambda})$$

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

$$k_0 = (\text{slope/intercept})(k_d + k_A[A]_0)$$
 (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 $\it I$ to $\it 6$ together with the reaction $\it 15$

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

Application of the steady-state approximation gives

$$(r_{ox}^{Q})^{-1} = (I_{a} \phi_{T}^{O2} \gamma_{\Delta} \gamma_{r}^{A})^{-1} \times$$

$$(26)$$

$$(k_{QT}[Q]/k_{TO}[O_{2}] + 1)[1 + [A]^{-1}(\beta_{A} + k_{Q}[Q]/k_{A})]$$

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 occurrence 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, and ka

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

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

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 $\phi_T^{O2}\gamma_\Delta$ 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

$$\phi_{AO2} = \phi_T^{O2} \gamma_{\Delta} k_r^{A} [A] / k_d \qquad (28)$$

and measurement of ϕ_{AO2} together with a knowledge of ϕ_T^{O2} , 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.

$$-d[A]/dt = (d[^{1}O_{2}^{*}]/dt)[k_{r}^{A}[A]/(k_{d} + k_{A}[A])]$$
 (29)

which integrates to give

$$\beta_{A} \ln([A]_{0}/[A]_{m}) + [A]_{0} - [A]_{m} = \gamma_{A}^{A}[^{1}O_{2}^{*}]_{m}$$
 (30)

where $[^{1}O_{2}^{*}]_{\infty}$ 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 = β_A . In the presence of a quencher eq (30) becomes

$$(\beta_{A} + k_{0}[Q]/k_{A})(\ln[A]_{0}/[A]_{\infty} + \Delta[A]) = \gamma_{r}^{A}[^{1}O_{2}^{*}]_{\infty} (32)$$

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 ${}^{1}O_{2}^{*}$ so that $[{}^{1}O_{2}^{*}]_{\infty}$ can be replaced by the initial concentration of $(C_{6}H_{5}O)_{3}PO_{3}$, i.e. $[{}^{1}O_{2}^{*}]_{\infty} = [(C_{6}H_{5}O)_{3}PO_{3}]_{0}$ and γ_{r}^{Λ} 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 $O_2^*(^1\Sigma_{\mu}^+)$ will be rapidly quenched, probably to give ${}^{1}O_{2}*({}^{1}\Delta_{\omega})$ 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 [A₀] in the presence and absence of a quencher gives

$$k_{Q} = [k_{A}([A]_{\infty}^{Q} - [A]_{\infty}^{0}) + k_{d}\ln([A]_{\infty}^{Q}/[A]_{\infty}^{0})]/[Q]\ln([A]_{0}/[A]_{\infty}^{Q})$$
(33)

where $[A]_{\infty}^{\ \ 0}$ 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 ${}^{1}O_{2}*({}^{1}\Delta_{g})$ state by absorption at 1065 nm from a CW Nd YAG laser and ${}^{1}O_{2}*({}^{1}\Delta_{g})$ 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 $\Phi_{\rm T}^{02}\gamma_{\Delta}$ by n=1 or 2 for excitation at 1065 nm or 633 nm respectively gives

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

and plots of ϕ_{A02}^{-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
$$2 {}^{3}O_{2}({}^{3}\Sigma_{g}^{-}) + h\nu \rightarrow {}^{1}O_{2}*({}^{1}\Delta_{g}) + {}^{3}O_{2}({}^{3}\Sigma_{g}^{-})$$

eq (14) has been modified by them to give

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

where E is the laser intensity and σ the absorption cross section for process 16. At high oxygen concentration where $k_{02}[O_2] > > (k_d + k_{\Lambda}[A])$ the observed first order rate constant k_1 is given by

$$k_1 = \sigma E[O_2]k_r^A/k_{O2}.$$
 (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

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

and a plot of ($[O_2]/k_1$) vs ($[Q]/[O_2]$) will have a slope/intercept = k_0/k_{02} .

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^{Λ} may be low by up to an order of magnitude.

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 $k_{\rm d}$ in various solvents, usually at an unspecified temperature, which from the few studies of temperature dependence of $k_{\rm d}$ (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 CCl4 (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 ± 10%. However the discrepancies between the values of $k_{\rm d}$ 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 $k_{\scriptscriptstyle d}$ the more critical is solvent purity. However the direct technique for measuring $k_{\rm d}$ depends on measuring $k_{\rm D}$ 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 $k_{\rm d}$ 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 $k_{\rm d}$ 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

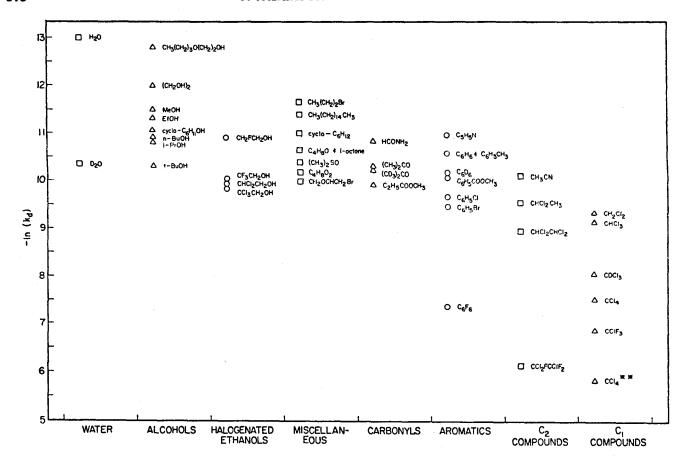


FIGURE 2. Plot of $-\ln(k_d)$ versus solvent class where k_d is the psuedo first order rate constant for physical deactivation of singlet oxygen by solvent molecules. ** Krasnovsky's value.

special comments. The method he uses is very direct since he measures emission from $O_2^*(^1\Delta_a)$. 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 (~ 50 times) for singlet oxygen in CCl4 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 $\leq \mu M$ 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 $k_d \leq 10^2 \text{ s}^{-1}$. Krasnovsky [40] has measured singlet oxygen quenching rate constants of 10^6 and 4×10^7 dm³ mol-1 s-1 respectively for tetraphenylporphine (TPP) and Zn²⁺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 10⁵ dm³ mol⁻¹ s⁻¹ (Even benzene, methanol and H₂O have quenching constants of about 3, 2 and $9 \times 10^3 \, \mathrm{dm}^3$ mol⁻¹ s⁻¹, respectively).

In the case of solvents where $k_{\rm d} \leq 10^2~{\rm s}^{-1}$, substantial quenching of singlet oxygen would be expected for sensitizer concentrations $> 10^{-4}~{\rm mol~dm}^{-3}$, and this could account for the different values of $k_{\rm d}$ reported by different

research groups. Thus independent evaluation 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 $k_{\rm d} \geq 10^2~{\rm s}^{-1}$. 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 CCl₄ however since the major application of $k_{\rm d}$ is to determine values of $k_{\rm A}$ or $k_{\rm O}$ and since most photo-oxygenation studies have used sensitizers it follows that the value required for deriving k_A or k_0 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 $k_{\rm d}$ 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 $k_{\rm D}$ determined. Quenching by the co-solvent is then allowed for effectively by taking

$$k_{\rm D} = k_{\rm d}({\rm sol})X_{\rm sol} + k_{\rm d}({\rm co-sol})X_{\rm co-solvent} + k_{\rm A}[{\rm A}]_{\rm av}$$
 (38)

where $X_{\rm sol}$ 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 $k_{\rm d}$ (co-sol), the decay constant in the neat co-solvent. Young and Brewer [64] have measured $k_{\rm co-solvent}$, 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),

$$k_{\text{co-solvent}} = k_{\text{d}}(\text{co-solvent})/[\text{neat co-solvent}]$$
 (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 $k_{\rm D}$ values determined in the presence of a small proportion of co-solvent to obtain a value of $k_{\rm d}$ 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 $10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ or that $k_0(\beta\text{-carotene})$ 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)₃PO₃ decomposition and from the self-photosensitization of rubrene in dichloromethane, Carlsson et al. [63] obtained estimates of 7.3 × 10^3 s^{-1} and $9.5 \times 10^3 \text{ s}^{-1}$, respectively, for the singlet oxygen decay constant in dichloromethane by assuming $k_{\rm A}$ (rubrene) = 7.3 \times 10⁷ dm³ mol s⁻¹. These values fall between the decay constants measured following pulsed excitation given in table 1 which are $7.1 \times 10^3 \, \mathrm{s}^{-1}$ and 1.6 × 10⁴ 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 ${}^{1}O_{2}^{*}$ decay in terms of electronic to solvent vibrational energy transfer, have shown that

$$k_d/10^6 \text{ s}^{-1} \approx 0.5 A_{7880} + 0.05 A_{6280}$$
 (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 $0\longrightarrow 0$ and $0\longrightarrow 1$ vibrational components for $O_2(^3\Sigma_g^-)\longleftarrow O_2*(^1\Delta_g)$ 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

$$\ln k_{\rm d} = (41)$$
 a + b[Ionization Potential/(0.5 A_{7880} + 0.05 A_{6280})]

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 .

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, or k_a 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 $k = 4.3 \times 10^4$ dm³ mol⁻¹ s⁻¹ using $k_{\rm d} = 3.8 \times 10^4 \, {\rm s}^{-1}$ and *3.5 $\times 10^4$ dm³ mol⁻¹ s⁻¹ if the preferred value $k_{\rm d}$ (Av) = *3.1 \times 10⁴ 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 kwith 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 dm³ 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 ± 1.3) $\times 10^8$ to $(1.5 \pm 0.5) \times 10^9$ dm³ 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

$${}^{1}O_{2}^{*} + {}^{1}Q \rightarrow {}^{3}Q^{*} + {}^{3}O_{2}$$

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:

$$^{1}O_{2}^{*} + NR_{3} \rightleftarrows$$
 $^{1}(O^{\delta-}...NR^{\delta+}) \rightleftarrows ^{3}(O^{\delta-}...NR^{\delta+}) \rightarrow ^{3}O_{2} + NR_{3}.$

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 O₂, neither does quenching by paramagnetic species, which could arise from the catalysed intersystem crossing process

$${}^{1}O_{2}^{*} + {}^{m}Q \rightarrow {}^{3}O_{2} + {}^{m}Q$$

which is spin allowed by Wigners Spin rule, give rise to efficient quenching since for example $k_{\rm q} \leq 10^4~{\rm dm}^3~{\rm mol}^{-1}~{\rm s}^{-1}$ for quenching of ${}^1{\rm O}_2*$ by ${}^3{\rm O}_2$ (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 $^{1}O_{2}^{*}$ 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)
$$\text{Et}_2S + {}^1O_2^* \to \text{Et}_2SOO \ (+ \text{Et}_2S) \to 2\text{Et}_2SO$$

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

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 | 2M2P TMHP | 2-methyl-2-pentene 2,2,6,6-tetramethyl-4-hydroxypiperidine |
|-------------------------------|---|--|--|
| General | | Substrate colu | mn |
| General | | TBA | tetrabutylammonium ion |
| S | sensitizer | TOS | p-toluenesulfonate ion |
| A | primary substrate | | |
| A' | reference substrate | Chemical grou | ups |
| A'' | second reference substrate | 9 ** | 1- |
| P | product of primary substrate | Me- | $\mathrm{CH_3}$ |
| P' | product of reference substrate | Et- | CH ₂ CH ₃ |
| ¹ O ₂ * | singlet oxygen | n-Pr- | CH ₂ CH ₂ CH ₃ |
| | • | i-Pr- | CH(CH ₃) ₂ |
| Sensitizers | | n-Bu- | $CH_2(CH_2)_2CH_3$ |
| | | s-Bu- | CH(CH ₃)CH ₂ CH ₃ |
| An | anthracene | t-Bu- | C(CH ₃) ₃ |
| azine | 3H-2-pivaloyl-4-phenyl-6-diethylamino- | Ph- | C_6H_5 |
| | 8-methylquinoxal-3-one | dtc | dithiocarbamate |
| BA | 1,2-benzanthracene | acac | acetylacetonate |
| BP | benzophenone | | , |
| DMA | 9,10-dimethylanthracene | Solvent colum | n |
| DNT | dinaphthalene thiophene | | |
| Eos | eosin | (5:1) v:v | 5 parts to 1 part by volume |
| Ery | erythrosine | <i>i</i> -octane | 2,2,4-trimethylpentane |
| FMN | riboflavin-5'-phosphate (flavine mononucleotide) | THF | tetrahydrofuran |
| MB | methylene blue | Rate data col | umns |
| MP | meso-porphyrin | | |
| Naph | naphthalene | k_{\star}^{A} | rate constant for chemical reaction of A |
| Per | perylene | $egin{array}{c} k_{r}^{\;A} \ oldsymbol{eta}_{r}^{\;A} \ k_{q}^{\;\;A} \ oldsymbol{eta}_{q}^{\;\;A} \end{array}$ | beta value for chemical reaction of A |
| Phen | phenanthrene | k_{σ}^{A} | rate constant for physical quenching of ${}^1\mathrm{O}_2{}^*$ |
| PP | protoporphyrin | β'n | beta value for physical quenching of 1O_2* |
| Py | pyrene | k | rate constant including both k_r^A and $k_q^{A^2}$ |
| RB | rose bengal | | components |
| RBCE | rose bengal complexed with | β | beta value including both β_r^A and β_q^A |
| • | dicyclohexyl-18-crown-6 | | components |
| Rub | rubrene | k_d | rate constant for solvent deactivation |
| self | self sensitization | $k_{ m D}$ | $(k_{d} + k_{A}[A])$ |
| Tetr | tetracene | $k_{\mathrm{Td}}^{}}$ | rate constant for substrate quenching of |
| TPP | tetraphenylporphine | | sensitizer triplets |
| ZnTPP | zinc tetraphenylporphine | (est) | estimated from an experimentally determined quantity |
| Reference subst | crates | | |
| | | Temperature o | column |
| Car | all trans-β-carotene | | |
| DABCO | 1,4-diazabicyclooctane | rt | temperature not reported, possibly room |
| <i>p</i> -dioxene | 3,6-dioxacyclohexene | | temperature |
| DDM | diazodiphenylmethane | Methods colu | mn |
| DMA | 9,10-dimethylanthracene | | |
| DMBA | 9,10-dimethyl-1,2-benzanthracene | Od- | rate monitored by oxygen disappearance |
| DPBF | 1,3-diphenylisobenzofuran | Ad~ | rate monitored by substrate disappearance |
| DPF | 2,5-diphenylfuran | A'd- | rate monitored by reference substrate |
| Rub | rubrene | | disappearance |
| TMS | trimethylstyrene | Pa- | rate monitored by product appearance |
| 2M2B | 2-methyl-2-butene | P'a- | rate monitored by reference product |
| TME | 2,3-dimethyl-2-butene | | appearance |
| # 74##7 | (tetramethylethylene) | Ld~ | rate monitored by ${}^{1}O_{2}^{*}$ luminescence decay |

Comments column

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

References to Text

- [1] Raab, O., Z. Biol. 39: 524 (1900).
- [2] Straub, W., Arch. Exptl. Pathol. Pharmakol. 51: 383 (1904).
- [3] Hausmann, W., Biochem. Z. 14: 275 and 15: 12 (1908).
- [4] Kautsky, H., de Bruijn, H., Naturwissenschaften 19: 1043 (1931).
- [5] Kautsky, H., de Bruijn, H., Neuwirth, R., Baumeister, W., Chem. Ber. 66B: 1588-1600 (1933).
- [6] Foote, C.S., Wexler, S., J. Am. Chem. Soc. 86: 3879-80, 86: 3880-1 (1964).
- [7] Corey, E.J., Taylor, W.C., J. Am. Chem. Soc. 86: 3881 (1964).
- [8] Schaap, P.A., Chapter 6, Singlet Oxygen, Monograph in Organic-Chemistry Series, H.H. Wasserman and R.W. Murray (eds.), Academic Press, New York, 1979, p.173-286 [79Z110].
- [9] Foote, C.S., Free Radicals in Biology. Volume 2., W.A. Pryor (ed.), Academic Press, New York, 1976, p.85-133 [76R101].
- [10] Spikes, J.D., Livingston, R., Adv. Radiat. Biol. 3: 29 (1969).
- [11] Wallis, C., Melnick, J.L., Photochem. Photobiol. 4: 159 (1965).
- [12] Blum, H.F., Photodynamic Action and Diseases Caused by Light, Hofher (1966).
- [13] Cleve, N.T., Radiation Biology, A. Hollaender (ed.), vol. 3, p.693, McGraw-Hill (1956).
- [14] Fitzpatrick, T.B., et al. (eds.), Dermatology in General Medicine, McGraw-Hill (1971).
- [15] Koka, P., Song, P.-S., Photochem. Photobiol. 28(4-5): 509-15 (1978) [78F404].
- [16] Goldstein, B.C., Hanher, L.C., J. Clin. Invest. 51: 892 (1972).
- [17] Trozzolo, A.M., Winslow, F.H., Macromolecules 1: 98 (1968).
- [18] Carlsson, D.J., Suprunchuk, T., Wiles, D.M., J. Polym. Sci., Polym. Lett. Ed. 11(1): 61-5 (1973) [73P066].
- [19] Kaplan, M.L., Kelleher, P.G., Rubb. Chem. Tech. 45: 423 (1972).
- [20] Rabek, J.F., Ranby, B., Polym. Eng. Sci. 15: 40 (1975).
- [21] Pitts, J.N., Jr., Khan, A.U., Smith, E.B., Wayne, R.P., Environ. Sci. Technol. 3: 241 (1969).
- [22] Khan, A.U., Kasha, M., Ann. New York Acad. Sci. 171: 24 (1970).
- [23] Bergsmer, D., Hsia, D.Y.Y., Jackson, C., Bilirubin Metabolism in the Newborn, Williams and Wilkins, (1970).
- [24] Dougherty, T.J., Abstracts for the International Conference on Singlet Oxygen and Related Species in Chemistry and Biology, Pinawa, Manitoba, Canada, 21-26 August 1977.
- [25] Backstrom, H.L.J., The Svedberg, Tiselius and Pedersen (eds.), p.45-64, Almqvist and Wiksell, Uppsula (1944).
- [26] Usui, Y., Itoh, K., Koizumi, M., Bull. Chem. Soc. Jpn. 38: 1015 (1965).
- [27] Wilkinson, F., J. Phys. Chem. 66: 2569 (1966).
- [28] Higgins, R., Foote, C.S., Cheng, H., Adv. Chem. 77: 102-17 (1968) [68F292].

- [29] Schenk, G.O., Koch, E., Z. Electrochem. 64: 170 (1960).
- [30] Gollnick, K., Adv. Photochem. 6: 1 (1968).
- [31] Kearns, D.R., Chem. Rev. 71: 395 (1971)[71F313].
- [32] Stevens, B., Acc. Chem. Res. 6: 90-6 (1973) [73F659].
- [33] Shlyapintokh, V.Ya., Ivanov, V.B., Russ. Chem. Rev. 45(2): 99– 110 (1976) [76F851].
- [34] Foote, C.S., Denny, R.W., Weaver, L., Chang, Y., Peters, J., Ann. New York Acad. Sci. 171: 139-45 (1970) [70F734].
- [35] Singlet Oxygen, Monograph in Organic Chemistry Series, H.H. Wasserman, R.W. Murray (eds.), Academic Press, New York, 1979.
- [36] International Conference on Singlet Oxygen and Related Species in Chemistry and Biology, Pinawa, Manitoba, Canada, 21-26 August 1977, Photochem. Photobiol. 28(4-5) (1978).
- [37] Childe, W.H., Mecke, R., Z. Physik 68: 344 (1971).
- [38] Wallace, L., Hunten, D.M., J. Geophys. Res. 73: 4813 (1968).
- [39] Krasnovsky, A.A., Biofizika 21: 748 (1976).
- [40] Krasnovsky, A.A., Jr., Photochem. Photobiol. 29(1): 29-36 (1979) [79A010].
- [41] Adams, D.R., Wilkinson, F., J. Chem. Soc., Faraday Trans. 2 68(4): 586-93 (1972) [72F126].
- [42] Merkel, P.B., Kearns, D.R., Chem. Phys. Lett. 12(1): 120-2 (1971) [71M325].
- [43] Merkel, P.B., Kearns, D.R., J. Am. Chem. Soc. 94(21): 7244-53 (1972) [72F260].
- [44] Young, R.H., Brewer, D., Keller, R.A., J. Am. Chem. Soc. 95(2): 375-9 (1973) [73F014].
- [45] Matheson, I.B.C., Lee, J., Yamanashi, B.S., Wolbarsht, M.L., J. Am. Chem. Soc. 96(11): 3343-8 (1974) [74F102].
- [46] Farmilo, A., Wilkinson, F., Photochem. Photobiol. 18(6): 447-50 (1973) [73F438].
- [47] Wilkinson, F., Singlet Oxygen, Reactions with Organic Compounds and Polymers, B. Ranby and J.F. Rabek (eds.), John Wiley, New York, N.Y., 1976, p.27-35 [76F902].
- [48] Wilkinson, F., Ho, W.-T., Spectrosc. Lett. 11(7): 455-63 (1978) [78F276].
- [49] Young, R.H., Wehrly, K., Martin, R.L., J. Am. Chem. Soc. 93(22): 5774-9 (1971) [71F398].
- [50] Young, R.H., Martin, R.L., Chinh, N., Mallon, C., Kayser, R.H., Can. J. Chem. 50: 932-8 (1972) [72F510].
- [51] Thomas, M.J., Foote, C.S., Photochem. Photobiol. 27(6): 683-93 (1978) [78A171].
- [52] Greenstock, C.L., Wiebe, R.H., Photochem. Photobiol. 28(4-5): 863-7 (1978) [78N003].
- [53] Foote, C.S., Chang, Y.C., Denny, R.W., J. Am. Chem. Soc. 92(17): 5216-8 (1970) [70F188].
- [54] Schenck, G.O., Gollnick, K., Neumueller, O.A., Ann. Chem. 603: 46-59 (1957) [57F008].
- [55] Tanielian, C., Chaineaux, J., J. Photochem. 9(1): 19-32 (1978) [78A344].
- [56] Mendenhall, G.D., Ph.D Thesis, Harvard, 1970 (see ref. 57).
- [57] Carlsson, D.J., Mendenhall, G.D., Suprunchuk, T., Wiles, D.M., J. Am. Chem. Soc. 94(25): 8960-2 (1972) [72F319].
- [58] Evans, D.F., Chem. Commun. 397 (1969).
- [59] Evans, D.F., Tucker, J.N., J. Chem. Soc., Faraday Trans. 2 72(9): 1661-6 (1976) [76F417].
- [60] Jori, G., Cauzzo, G., Photochem. Photobiol. 12: 231-7 (1970) [70F732].
- [61] Matheson, I.B.C., Lee, J., J. Am. Chem. Soc. 94(10): 3310-3 (1972) [72F513].
- [62] Matheson, I.B.C., Toledo, M.M., Photochem. Photobiol. 25(3): 243-8 (1977) [77F129].
- [63] Carlsson, D.J., Suprunchuk, T., Wiles, D.M., Can. J. Chem. 52(22): 3728-37 (1974) [74F341].
- [64] Young, R.H., Brewer, D.R., Singlet Oxygen, Reactions with Organic Compounds and Polymers, B. Ranby and J.F. Rabek (eds.), John Wiley, New York, N.Y., 1976, p.36-47 [76F903].
- [65] Merkel, P.B., Kearns, D.R., J. Am. Chem. Soc. 94(3): 1029-30 (1972) [72F026].

- [66] Koch, E., Tetrahedron 24: 6295-318 (1968) [68F288].
- [67] Young, R.H., Martin, R.L., J. Am. Chem. Soc. 94(15): 5183-5 (1972) [72F514].
- [68] Furukawa, K., Ogryzlo, E.A., J. Photochem. 1(2): 163-9 (1972) [72E210].
- [69] Ouannes, C., Wilson, T., J. Am. Chem. Soc. 90(23): 6527-8 (1968) [68F285].
- [70] Smith, W.F., Jr., Herkstroeter, W.G., Eddy, K.L., J. Am. Chem. Soc. 97(10): 2764-70 (1975) [75F166].
- [71] Young, R.H., Brewer, D., Kayser, R., Martin, R., Feriozi, D., Keller, R.A., Can. J. Chem. 52: 2889-93 (1974) [74F640].
- [72] Foote, C.S., Singlet Oxygen, H.H. Wasserman and R.W. Murray (eds.), Academic Press, New York, N.Y., 1979, p.139– 173[79Z109].

CHEMICAL KINETICS OF SINGLET OXYGEN IN SOLUTION

TABLE 1. Decay constants of singlet oxygen in various solvents

| No. | Solvent | $k_{\rm d}/{\rm s}^{-1}$ | t/°C | Comments | Ref. |
|----------------|---|---|------|---|-------------|
| 1.1 | H₂O (water) | $\ddagger (5.0 \pm 2.0) \times 10^5$ | rt | S = MB, $A = DPBF$, ruby laser (694 nm). k_d extrapolated from a value in | Merk.72F026 |
| 1.1.1 | | ‡4.8 x 10 ⁵ | rt | $(H_2O/MeOH)$ (1:1) v:v mixture. S = MB, $A = DPBF$, dye laser (610 nm). k_d corrected to zero MeOH concentration. | Youn.76F903 |
| 1.1.2 | , | ‡3.3 x 10 ⁵ | rt | S = 2-acetonaphthone, A = DPBF, nitrogen laser (337 nm).DPBF solubilized in SDS micelles in air saturated H ₂ O solutions. | Gorm.78E144 |
| 1.1.3 | | $(x) = *4.4 \times 10^5$ | | | |
| 1.2 | D_2O (water- d_2) | $\ddagger (3.0 \pm 0.2) \times 10^4$ | 20 | S = MB, $A = DPBF$, dye laser (620 nm). k_d determined in air saturated D_2O solutions of DPBF solubilized in SDS micelles. | Math78E143 |
| 1.2.1 | | $\ddagger (2.8 \pm 0.2) \times 10^4$ | 20 | S = MB, A = DPBF, dye laser (620 nm). k_d determined in air saturated D ₂ O solutions of DPBF solubilized in CTAB micelles. | Math78E143 |
| 1.2.2 | | ‡3.3 x 10 ⁴ | rt | S = 2-acetonaphthone, A = DPBF, nitrogen laser (337 nm). DPBF solubilized in SDS micelles in air saturated D ₂ O solutions. | Gorm.78E144 |
| 1.2.3 | | $(x) = *3.1 \times 10^4$ | | • | |
| 1.3 | CH ₃ OH (methanol) | $(1.4 \pm 0.2) \times 10^5$ | rt | S = MB, A = DPBF, ruby laser (694 nm). | Merk.71M325 |
| 1.3.1 | | $\leq (2.0 \pm 0.2) \times 10^5$ | 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 | | $1(8.8 \pm 0.4) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn73F014 |
| 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. | Youn73F014 |
| 1.3.4 | | $t(1.1 \pm 0.2) \times 10^{5}$ | rt | S = MB, $A = DPBF$, ruby laser (347 nm). | Wilk76F902 |
| 1.3.5 | 1. / A | \$1.1 x 10 ⁵ | 25 | S = MB, $A = DPBF$, ruby laser (694 nm). | Usui78F061 |
| 1.3.6 1.4 | CH ₂ Cl ₂ (dichloromethane) | $0) = *(1.0 \pm 0.2) \times 10^{5}$ 11.6×10^{4} | 25 | S = MB, A = DPBF, ruby laser (694 nm). | Usui78F061 |
| 1.4.1 1.4.2 | , | 17.1×10^{3} $= *1.2 \times 10^{4}$ | rt | S = MB, $A = DPBF$, dye laser (610 nm). | Youn.76F903 |
| 1.5 | CHCl ₃ (chloroform) | $1(1.7 \pm 0.4) \times 10^4$ | 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 | | $t(4.4 \pm 1.8) \times 10^3$ | rt | S = MB, $A = DPBF$, dye laser (610 nm). | Youn.76F903 |
| 1.5.2 1.5.3 | k (Av | \$\$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ \$ | 25 | S = MB, $A = DPBF$, ruby laser (694 nm). | Usui78F061 |
| 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 ₃ Cl (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 tetra- chloride) | $\ddagger (1.4 \pm 0.7) \times 10^3$ | rt | S = MB, $A = DPBF$, ruby laser (694 nm). k_d corrected for 2% MeOH content. | Merk.72F260 |
| 1.8.1 | , | ‡2.2 x 10 ³ | rt | S = MB, $A = DPBF$, dye laser (610 nm). | Youn.76F903 |
| 1.8.2 | | $1(1.42 \pm 0.40) \times 10^3$ | 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 x 10 ¹ | rt | using k_d values for CC ₁ /MeOH mixtures (1-3% MeOH). $S = TPP, PP, MP, pheophytins. k_d$ from direct measure of decay of sensitized luminescence from ${}^{1}O_2*$ using a phosphoroscope. | Kras79A010 |
| 1.8.4 | • | $) = *1.7 \times 10^{3}$ | | | |
| 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. S = MB, A = DPBF, ruby laser (604 nm). | Merk.72F260 |
| 1.10 | CH ₃ CH ₂ OH (ethanol) | $\ddagger (8.3 \pm 1.7) \times 10^4$ | rt | S = MB, $A = DPBF$, ruby laser (694 nm). | Merk.72F260 |
| 1.10.1 | • | $\ddagger (1.0 \pm 0.1) \times 10^5$ | rt | S = MB, $A = DPBF$, ruby laser (347 nm). | Wilk76F902 |

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

| No. | Solvent | $k_{\rm d}/{ m s}^{-1}$ | t/°C | Comments | Ref. |
|----------------|--|--|------|---|---------------|
| 1.10.2 | | $\ddagger (5.3 \pm 0.9) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.10.3 1.11 | $k_d(Av) = HO(CH_2)_2OH$ (1,2-dihydroxy-ethane) | = *7.9 x 10 ⁴ 4.8 x 10 ⁵ | rt | S = MB or RB, A = DPBF, dye laser. $k_{\rm D} = 5.1 \times 10^5 \text{s}^{-1}$ when [DPBF] = 1.7 x 10 ⁻⁵ mol dm ⁻³ and $\beta = 3.2 \times 10^{-4}$ mol dm ⁻³ (for method see | Youn.73F014 |
| 1.11.1 | | *1.6 x 10 ⁵ | rt | section (4)). S = MB, $A = DPBF$, dye laser (610 nm). k_d corrected to zero MeOH concentration. k_d value very different from previous value | Youn.76F903 |
| 1.12 | CH₂FCH₂OH | $(5.6 \pm 1.2) \times 10^4$ | rt | of same authors [73F014]. S = MB, A = DPBF, dye laser (610 nm). | Youn.76F903 |
| 1.13 | (2-fluoroethanol) CH ₃ CHCl ₂ | 1.5 x 10⁴ | 25 | Error is a 90% confidence limit. S = MB, A = DPBF, ruby laser (694 nm). | Usui.:.78F061 |
| 1.14 | (1,1-dichloroethane) CHCl ₂ CH ₂ OH (2,2-dichloro- ethanol) | $(2.1 \pm 0.6) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.15 | CCl ₃ CH ₂ OH (2,2,2-trichloro- ethanol) | $(2.0 \pm 0.6) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.16 | CF ₃ CH ₂ OH (2,2,2-trifluoro- ethanol) | $(2.3 \pm 0.6) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.17 | CH ₃ CN (acetonitrile) | $\ddagger (3.3 \pm 0.7) \times 10^4$ | rt | S = MB, $A = DPBF$, ruby laser (694 nm). | Merk.72F260 |
| 1.17.1 | (accionitric) | $\ddagger (1.8 \pm 0.3) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90 % confidence limit. | Youn.76F903 |
| 1.17.2 | $k_{\rm d}({\rm Av}) =$ | *2.55 x 10 ⁴ | | | |
| 1.18 | CHCl ₂ CHCl ₂ (1,1,2,2-tetra-chloroethane) | 8.3 x 10 ³ | 25 | S = MB, $A = DPBF$, ruby laser (694 nm). | Usui78F061 |
| 1.19 | CH ₃ CHOHCH ₃ (2-propanol) | $(5.0 \pm 0.3) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.20 | CH ₃ (CH ₂) ₂ Br (1-bromopropane) | $1(1.0 \pm 0.2) \times 10^5$ | rt | S = MB, $A = DPBF$, ruby laser (347 nm). | Wilk76F902 |
| 1.20.1 | (1 etemop-opune) | $\ddagger (1.3 \pm 0.4) \times 10^5$ | 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 |
| 1.20.2 | | *1.15 x 10 ⁵ | | | |
| 1.21 | HCON(CH ₃) ₂ (dimethyl- formamide) | $\leq (1.4 \pm 0.1) \times 10^5$ | 23 | $S = An, Phen, Py, BA; A = DPBF, ruby laser (347 nm). Value not corrected for a k_i[DPBF] contribution. Error is a standard deviation.$ | Adam.72F126 |
| 1.22 | CH ₃ COCH ₃ (acetone) | $\ddagger (3.8 \pm 0.8) \times 10^4$ | rt | S = MB, A = DPBF, ruby laser (694 nm). | Merk.72F026 |
| 1.22.1 | | $\ddagger (2.4 \pm 0.5) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.22.2 | | *3.1 x 10 ⁴ | | | |
| 1.23 | CH ₂ OCHCH ₂ Br (1-bromo-2,3-epoxy- propane) | $(2.2 \pm 0.5) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.24 | CH ₃ (CH ₂) ₃ OH (1-butanol) | $(5.2 \pm 0.8) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn73F014 |
| 1.25 | (CH ₃) ₃ COH (2-methyl-2- propanol) | $(3.0 \pm 0.4) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn73F014 |
| 1.26 | C ₄ H ₈ O (tetrahydrofuran) | $(4.3 \pm 0.4) \times 10^4$ | rt | S = RB, A = DPBF, dye laser (583 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.27 | C ₄ H ₈ O ₂ (dioxane) | $(2.9 \pm 1.0) \times 10^4$ | rt | S = MB, $A = DPBF$, dye laser (610 nm). | Youn73F014 |
| 1.28 | CH ₃ COOCH ₂ CH ₃ (ethyl acetate) | $(2.1 \pm 0.7) \times 10^4$ | rt | Error is a 95% confidence limit. S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.29 | C ₅ H ₅ N (pyridine) | $(3.1 \pm 1.4) \times 10^4$ | 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 | $k_{\rm d}/{\rm s}^{-1}$ | t/°C | Comments | Ref. |
|----------------|---|--|--------|--|-------------|
| 1.29.1 | | * $(5.9 \pm 1.4) \times 10^4$ | 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 ₆ H ₁₂ (cyclohexane) | $(5.9 \pm 0.2) \times 10^4$ | rt | S = MB, $A = DPBF$, ruby laser (694 nm). k_d corrected for 2% MeOH content. | Merk.72F260 |
| 1.31 | C ₆ H ₁₁ OH (cyclohexanol) | $(6.3 \pm 0.9) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.32 | C ₆ H ₆ (benzene) | $\ddagger (4.2 \pm 0.9) \times 10^4$ | rt | S = MB, $A = DPBF$, ruby laser (694 nm). | Merk.72F026 |
| 1.32.1 | (ochzenc) | $\leq (8.0 \pm 0.5) \times 10^4$ | 23 | S = Naph,BP,An,Phen,Py,BA; A = DPBF, ruby laser (347 nm). Value not corrected for a k_1 [DPBF] contribution. For revised value see [73F438]. Reported error is a standard deviation. | Adam.72F126 |
| 1.32.2 | | $<(7.0 \pm 1.0) \times 10^4$ | 23 | S = BA, A = DPBF, ruby laser (347 nm). Value not corrected for k _i [DPBF] contribution. For revised value see [73F438]. Reported error is a standard deviation. | Adam.72F126 |
| 1.32.3 | | $<(8.0 \pm 2.0) \times 10^4$ | 5 | S = BA, A = DPBF, ruby laser (347 nm). Value not corrected for k ₁ [DPBF] contribution. For revised value see [73F438]. Reported error is a standard deviation. | Adam.72F126 |
| 1.32.4 | | $t(3.9 \pm 0.4) \times 10^4$ | rt | S = An, $A = DPBF$, ruby laser (347 nm). | Farm.73F438 |
| 1.32.5 | | $\ddagger (4.1 \pm 0.3) \times 10^4$ | 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 | | $1(3.7 \pm 0.6) \times 10^4$ | 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. | Gorm78E263 |
| 1.32.8 | | $\ddagger (4.1 \pm 0.4) \times 10^4$ | 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 | $k_{\rm d}({ m Av})$ | $= *(4.0 \pm 0.7) \times 10^4$ | | , | |
| 1.33 | C_6D_6 (benzene- d_6) | $(2.8 \pm 0.6) \times 10^4$ | rt | S = MB, $A = DPBF$, ruby laser (347 nm). | Wilk76F902 |
| 1.34 | C ₆ H ₅ Br (bromobenzene) | $(1.3 \pm 0.6) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.35 | C ₆ F ₆ (hexafluoro- benzene) | $(1.7 \pm 0.6) \times 10^3$ | rt | $S = MB$, $A = DPBF$, ruby laser (694 nm). k_d corrected for 1-2% MeOH content. | Long.75F088 |
| 1.36 | C ₆ H ₅ CH 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. | Gorm78E263 |
| 1.37 | C ₆ H ₅ COOCH ₃ (methyl benzoate) | $(2.5 \pm 1.0) \times 10^4$ | rt | S = MB, A = DPBF, dye laser (610 nm). Error is a 90% confidence limit. | Youn.76F903 |
| 1.38 | H ₂ O/CH ₃ OH (1:1) v:v | ‡2.9 x 10 ⁵ | rt | S = MB, A = DPBF, ruby laser (694 nm). | Merk.72F027 |
| 1.38.1 | | $1(2.8 \pm 0.8) \times 10^5$ | rt | S = MB or RB, A = DPBF, dye laser. $k_{\rm D} = 3.7 \times 10^5 {\rm s}^{-1}$ when [DPBF] = 1.7 x 10 ⁻⁵ mol dm ⁻³ and $\beta = 5.5 \times 10^{-5}$ mol dm ⁻³ (for method see section (5)). | Youn73F014 |
| 1.38.2 1.39 | D ₂ O/CH ₃ OH | $0 = *2.9 \times 10^5$ 9.1×10^4 | rt | S = MB, A = DPBF, ruby laser (694 nm). | Merk.72F027 |
| 1.40 | (1:1) v:v CH ₃ OH /HO(CH ₂) ₂ OH (1:1) v:v | $(1.2 \pm 0.2) \times 10^5$ | rt | S = MB or RB, A = DPBF, dye laser. $k_{\rm D} = 1.6 \times 10^5 {\rm s}^{-1} {\rm when} [{\rm DPBF}] = 1.9 \times 10^{-5} {\rm mol} {\rm dm}^{-3} {\rm and} \beta = 6.3 \times 10^{-5} {\rm mol} {\rm dm}^{-3} ({\rm for} {\rm method} {\rm mol} {\rm cm}^{-3} ({\rm mol} {\rm cm}^{-3}) $ | Youn73F014 |
| 1.41 | CCl ₄ /CH ₃ OH (99:1) v:v | $(3.0 \pm 2.0) \times 10^3$ | 25 | see section (5)). 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 | $k_{\rm d}/{ m s}^{-1}$ | t/°C | Comments | Ref. |
|--------|---|---------------------------------------|------|---|-------------|
| 1.42 | CCl ₄ /CH ₃ OH (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 ₃ OH (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 ₃ OH (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 ₃ OH (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 ₃ OH (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. | Floo73F334 |
| 1.48 | CH ₃ CH ₂ OH/H ₂ O (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) x 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 $k_{\rm r}[DPBF]$ 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. | Youn73F014 |
| 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. | Youn73F014 |

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 | $k_{\rm d}/{\rm s}^{-1}$ | t/°C | Comments | Ref. |
|----------|---|--|------|---|-------------|
| l(a).0 | CH ₃ CH ₂ I | 2.5 x 10 ⁵ (est) | rt | k_d estimated using eq. (39) from text and $k_A(CH_3CH_2I) = 4 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [15.4].$ | Wilk76F902 |
| l(a). l | (CH ₃) ₂ SO (dimethylsulfoxide) | 5.2 x 10 ⁴ *3.4 x 10 ⁴ (est) | rt | $S = RB$, $A = DPBF$, $A' = 2M2P$. Measured $\beta_{A'} = (5.5 \pm 0.1) \times 10^{-2} \text{ mol dm}^{-3}$, assumed $k_{A'} = 9.38 \times 10^5 (*6.25 \times 10^5) \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ (value in MeOH from } [2.40.2]).$ | Guir.76E072 |
| l(a).1.1 | | 3.33 x 10 ⁴ (est) | rt | Method not reported, may be direct method given in ref. [71M325]. | Nils.74F643 |
| (a).2 | CCl ₂ FCClF ₂ (Freon-113) | 4.3 x 10 ² (est) | rt | A = Rub. k_d estimated from β_A (Freon-113) = 1.1 x 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 |
| (a).2.1 | | 5.0 x 10 ² (est) | rt | A = DPBF. k_d estimated from β_A (Freon-113) = 5.4 x 10 ⁻⁷ mol dm ⁻³ assuming $k_A = 9.2$ x 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ where k_A is an average of all values listed under entry 5.36. | Stev76F905 |
| (a).3 | $(CD_3)_2CO$ (acetone- d_6) | 3.8 x 10 ⁴ *3.1 x 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 $k_d((CH_3)_2CO) = 3.8 \times 10^4 (*3.1 \times 10^4) \text{ s}^{-1}$ [1.22]. | Merk.72F260 |
| (a).4 | CH ₃ (CH ₂) ₃ O(CH ₂) ₂ OH (2-butoxyethanol) | 3.8 x 10 ⁵ (est) | 0 | A = Rub, Q = DABCO, $^{1}O_{2}^{*}$ from microwave discharge. Assumed $k_{Q} = 3.4 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{A} = 7.0 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and used equation (33). | Carl72F319 |
| (a).5 | C ₆ H ₃ Cl (chlorobenzene) | 1.6 x 10 ⁴ (est) | 25 | S = TPP, A = 3-methyl-2-pentene. The authors assumed $k_A = 1.0 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. However they give $\beta_A = 1.64 \times 10^{-2} \text{ mol dm}^{-3}$ in the text and $\beta_A = 1.6 \times 10^{-4} \text{ mol dm}^{-3}$ in a table. Using these values with k_A gives estimates for k_d of $1.6 \times 10^4 \text{ s}^{-1}$ and $1.6 \times 10^2 \text{ s}^{-1}$ respectively. | Carl74F341 |
| (a).6 | (CH ₃) ₂ CHCH ₂ C(CH ₃) ₃ (2,2,4-trimethylpentane) (<i>i</i> -octane) | 4.0 x 10 ⁴ (est) | 25 | S = A = Rub, Q = DABCO. Assumed k_Q = 3.4 x 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ and k_A = 7 x 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ and used equation (23). | Carl72F31 |
| (a).6.1 | (r-octaile) | 4.7 x 10 ⁴ (est) | 25 | A = Rub, ${}^{1}O_{2}^{*}$ from (PhO) ₃ PO ₃ decomp. Measured $\beta_{A} = 6.4 \times 10^{-4} \text{ mol dm}^{-3}$, assumed $k_{A} = 7.3 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$. Solvent contained 5% by volume of both MeOH and $C_{5}H_{5}N$. | Carl74F341 |
| (a).7 | CH ₃ (CH ₂) ₁₄ CH ₃ (hexadecane) | 9.0 x 10 ⁴ (est) | 25 | A = Rub, ${}^{1}O_{2}^{*}$ from microwave discharge. Measured $\beta_{A} = 1.2 \times 10^{-3} \text{ mol dm}^{-3}$, assumed $k_{A} = 7.3 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and used equation (33). | Carl74F341 |
| (a).8 | D ₂ O/CD ₃ OD (1:1) v:v | 2.9 x 10 ⁴ (est) | rt | S = MB, A = DPBF. Measured r_{ox} in both H ₂ O/CH ₃ OH and D ₂ O/CD ₃ OD. Assumed k_A is insensitive to solvent composition and k_d (H ₂ O/CH ₃ OH) = $(2.9 \pm 0.5) \times 10^5 \text{ s}^{-1}$ [1.38.2]. | Merk72F02 |
| (a).9 | CH ₂ Cl ₂ /CH ₃ OH (11:5) v:v | 2.1 x 10 ⁴ (est) | rt | A = Rub, Q = cis- and trans-1,4-dicloro-1,4-dinitrosocyclohexane, ${}^{1}O_{2}$ * from (PhO) ₃ PO ₃ decomp. Assumed $k_{A} = 4.0 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$. | Sing.76F900 |
| (a).10 | CH ₂ Cl ₂ /CH ₃ OH (15:1) v:v | 1.1 x 10 ⁴ (est) | rt | A = Rub, Q = $(CH_3)_3CNO$, ${}^1O_2^*$ from $(PhO)_3PO_3$ decomp. Assumed $k_A = 4.0 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Sing.76F900 |
| l(a).11 | CH ₂ Cl ₂ /C ₅ H ₅ N/MeOH (93:3:3) v:v:v | 5.0 x 10 ⁴ (est) | 25 | A = Rub, Q = DABCO, ${}^{1}O_{2}^{*}$ from (PhO) ₃ PO ₃ decomp. Measured β_{A} = (unreported), assumed k_{A} = 7×10^{7} dm ³ mol ⁻¹ s ⁻¹ and used equation (30). | Carl72F319 |

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

| 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 re or k_q (quenchi | presents the overall ing rate constant) is | rate constant unless k_r (ch specified; k_d is the rate co | emical nstant | reaction ra for solvent | te constant) deactivation | |
| 2.1 ethoxyethene CH ₂ =CHOC ₂ H ₅ | (Me) ₂ CO | $k_r = 5.7 \times 10^4$ *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 × 10 ⁵ (*1.8 × 10 ⁵) dm ³ | Bart70F73 |
| 2.1.1 | (Me) ₂ CO | 4.3×10^4 $*3.5 \times 10^4$ | $(8.8 \pm 0.2) \times 10^{-1}$ | 15 | A'd-16 | mol ⁻¹ s ⁻¹ [2.55.1]. S = RB, A' = DPBF. k derived using $k_d = 3.8 \times 10^4$ | Fale77F876 |
| 2.1.2 | (Me)₂CO | $k_{\rm r} = 3.1 \times 10^4$ *2.5 × 10 ⁴ | | 6 | Ad-17 A'd | (*3.1 × 10 ⁴) s ⁻¹ [1.22]. S = RB, A' = p-dioxene. Measured (k_r/k_r^A) = 0.14 ± 0.03. k_r derived using $k_r^{A'}$ = 2.2 × 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 ₆ H 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) ₂ CO | $k_{\rm r} < 1 \times 10^4$ (est) | | 6 | Ad-17 A'd | S = RB, $A' = p$ -dioxene. No measurable reaction of A | Fale77F876 |
| 2.2.2 | C ₆ H ₆ | 2.6 × 10 ⁵ | $(1.5 \pm 0.1) \times 10^{-1}$ | 15 | | S = RBCE, A' = DPBF. k derived using $k_0 = 4.2 \times 10^4$ s ⁻¹ [1.32]. | Fale77F876 |
| 2.3 $cis-1,2-diethoxy-$ ethene $C_2H_5OCH=CHOC$ | | $k_{\rm r} = 3.3 \times 10^7$ *2.7 × 10 ⁷ | | 8 | ? | S = ?, $A' = p$ -dioxene. Measured $(k_r/k_r^A) = 151$. k_r derived using $k_r^A = 2.2 \times 10^5 (*1.8 \times 10^5) dm^3$ mol ⁻¹ s ⁻¹ [2.55.1]. | Bart70F73 |
| 2.3.1 | (Me) ₂ CO | 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 | $k_{\rm r} = 5.7 \times 10^7$ *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 × 10 ⁷ (*3.0 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [A3.2]. Found $k_r >> k_q$. | Fale77F876 |
| 2.4 $trans-1,2$ -diethoxy- ethene $C_2H_5OCH=CHOC$ | · (Me) ₂ CO | For more relative rate $k_{\rm r} = 1.0 \times 10^7$ $*8.3 \times 10^6$ | rs see 2.4.2. | 8 | ? | S = ?, A' = p-dioxene. Measured (k_r/k_r^A) = 46. k_r derived using k_r^A = 2.2 × 10 ⁵ (*1.8 × 10 ⁵) dm ³ mol ⁻¹ s ⁻¹ [2.55.1]. | Bart70F73 |
| 2.4.1 | (Me) ₂ CO | 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 $k_d = 3.8 \times 10^4$ $(*3.1 \times 10^4) \text{ s}^{-1}$ [1.22]. | Fale77F876 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|---|----------------------|--|---------------------------------------|----------|--------------|--|------------|
| 2.4.2 | | (Me)₂CO | $k_{\rm r} = 2.6 \times 10^7$ *1.5 × 10 ⁷ | | 6 | Ad-17 A'd | S = RB, A' = cis -1,2-diethoxyethene. Measured $(k_r/k_r^{A'})$ = 4.55×10^{-1} . k_r derived using $k_r^{A'}$ = 5.7×10^7 (*3.2 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [2.3.2]. | Fale77F876 |
| 2.5 | methylidene- cyclopentane | CH ₃ CN | $k_{\rm r}=4.6\times10^4$ | | rt | ? | S = MB, A' = 1-methyl- cyclohexene. 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]. | Jeff73F66 |
| 2.5.1 | | CH ₃ CN | $k_{\rm r}=5.6\times10^4$ | | 0 | Ad-17 A'd | S = MB, A' = 2-methyl-idenenorborn-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]. | Jeff78F149 |
| 2.6 | ethylidene- cyclopentane | CHCl ₃ | $(8.7 \pm 1.3) \times 10^6$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'}$ = 5.3×10^7 dm ³ mol ⁻¹ s ⁻¹ [3.63.3] and k_d = 1.67×10^4 s ⁻¹ [1.5]. | Monr78A00 |
| 2.7 | methylidene- cyclohexane | CH3CN | $k_{\rm r} < 1 \times 10^3$ (est) | | rt | ? | S = MB, A' = 1-methyl-cyclohexene. | Jeff73F66 |
| 2.8 | ethylidene- cyclohexane | CHCl ₃ | $(8.6 \pm 1.3) \times 10^5$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'}$ = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ $[3.63.3] \text{ and } k_{d}$ = $1.67 \times 10^4 \text{ s}^{-1} [1.5]$. | Monr78A00 |
| 2.9 | 1,1,2-triethoxy- ethene $C_2H_5OCH = C(OC)$ | . , , = | 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-tricyclo- propylethene | (Me) ₂ CO | $k_{\rm r}=5.2\times10^{\rm 5}$ | | rt | Ad-17 A'd | S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured $(k_r/k_r^{A'}) = 0.40. k_r$ derived using $k_r^{A'} = 1.3 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [2.19.4]. | Rous78F43 |
| 2.11 | (cyclopropylmethy idene)cyclobutane | | $k_{\rm r}=7.7\times10^5$ | | rt | Ad-17 A'd | Each $A' = (\text{dicyclo-propylmethylidene}) \text{cyclo-butane. Measured}$ $(k_r/k_r^{A'}) = 0.59. k_r$ $\text{derived using } k_r^{A'} = 1.3 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ $[2.19.4].$ | Rous78F43 |

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

| No. S | Substrate (A) | Solvent | /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|-------------------------------|--|---------------------------------------|----------|--------------|---|------------|
| 2.12 | 1,1,2,2-tetra- ethoxyethene (C ₂ H ₅ O) ₂ C=C(OC 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 $k_d = 1.7 \times 10^4$ $(*1.0 \times 10^4) s^{-1}$ [1.5]. Solvent | Fale77F876 |
| 2.12.1 | | CH ₃ CN | 4.3×10^{7} *3.3 × 10 ⁷ | $(7.69 \pm .04) \times 10^{-4}$ | 15 | A'd-16 | contained 1% EtOH. S = RB, A' = DPBF. k derived using $k_d = 3.3 \times 10^4$ | Fale77F876 |
| 2.12.2 | | (Me) ₂ CO | 4.5×10^{7} $*3.6 \times 10^{7}$ | $(8.5 \pm 0.1) \times 10^{-4}$ | 15 | A'd-16 | $(*2.55 \times 10^4) \text{ s}^{-1}$ [1.17]. S = RB, A' = DPBF. k derived using $k_d = 3.8 \times 10^4$ | Fale77F876 |
| 2.12.3 | | (Me) ₂ CO | $k_{\rm r} = 4.6 \times 10^7$ *2.6 × 10 ⁷ | | 6 | Ad-17 A'd | (*3.1 × 10 ⁴) s ⁻¹ [1.22]. S = RB, A' = TME. Measured $(k_r/k_r^{A'})$ = 0.854. k_r derived using $k_r^{A'}$ = 5.4 × 10 ⁷ (*3.0 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ | Fale77F876 |
| 2.12.4 | | C ₆ H ₆ | 7.4×10^7 | $(5.67 \pm .18) \times 10^{-4}$ | 15 | A'd-16 | [A3.2]. Found $k_r >> k_q$. 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 $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. | Goll62F005 |
| 2.13.1 | | МеОН | 3.3×10^{6} | 3.0×10^{-2} | 20 | Od-15 | using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a =$ | Koch68F28 |
| 2.14 | 2-cyclohexyl-idene-cyclohexanol | | 2.3×10^5 | 4.4 × 10 ⁻¹ | rt | ? | 5.4 kJ mol ⁻¹ . Method not given. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | Goll62F005 |
| 2.15 | 2-cyclohexyl-idene-cyclohexanon | | 2.7 × 10 ⁵ | 3.7×10^{-1} | rt | ? | Method not given. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. | Goll62F005 |
| 2.15.1 | | МеОН | 2.9 × 10 ⁵ | 3.5×10^{-1} | 20 | Od-15 | using $k_{\rm d} = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_{\rm a} =$ | Koch68F28 |
| 2.16 | $\Delta^{9,10}$ -octalin | CHCl ₃ | $(5.0 \pm 0.8) \times 10^6$ | | rt | A'd-33 | 11.7 kJ mol ⁻¹ . 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]. | Monr78A00 |

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

| No. S | ubstrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /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 \times 10 ⁴) s ⁻¹ [<i>I.5</i>]. Solvent contained 1% EtOH. | Fale77F876 |
| 2.18 | (dicyclopropyl-methylidene)cyclo-propane | (Me) ₂ CO | $k_{\rm r}=1.4\times10^6$ | | rt | Ad-17 A'd | S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured $(k_r/k_r^A) = 1.05$. k_r derived using $k_r^{A'} = 1.3 \times 10^6$ dm ³ mol ⁻¹ s ⁻¹ [2.19.4]. | Rous78F430 |
| 2.19 | (dicyclopropyl-methylidene)cyclo-butane | МеОН | $k_{\rm r}=1.1\times10^6$ | | 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]. | Rous78F430 |
| 2.19.1 | | CH ₂ Cl ₂ | $k_{\rm r}=1.1\times10^6$ | | 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]. | Rous78F430 |
| 2.19.2 | · | CS ₂ | $k_{\rm r}=1.1\times10^6$ | | 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 $k_r^{A'}$ = $5.0 \times 10^6 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [3.10]. | Rous78F430 |
| 2.19.3 | | CH₃CH₂I | $k_{\rm r}=1.1\times10^6$ | | 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]. | Rous78F430 |
| 19.4 | | (Me) ₂ CO | $k_{\rm r}=1.3\times10^6$ | | 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]. | Rous78F430 |
| .19.5 | | C ₆ H ₆ | $k_{\rm r}=1.3\times10^6$ | | rt | Ad-17 A'd | [5.10]. S = TPP, A' = TMS. Measured (k_r/k_r^A) = $(2.5 \pm 0.4) \times 10^{-1} k_r$ derived using $k_r^{A'}$ = $5.0 \times 10^6 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [3.10]. | Rous78F430 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|------|--|-----------------------------|--|---------------------------------------|----------|--------------|---|-------------|
| 2.20 | (dicyclopropyl-methylidene)cyclo-pentane | | $k_{\rm r}=1.2\times10^6$ | | rt | Ad-17 A'd | S = Eos, A' = (dicyclopropylmethylidene)cyclobutane. Measured $(k_r/k_r^{A'}) = 0.90$. k_r derived using $k_r^{A'} = 1.3 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [2.19.4]. | Rous78F430 |
| 2.21 | 2-methylpropene $(CH_3)_2C=CH_2$ | МеОН | 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 68F28 |
| 2.22 | 2-propenal CH ₂ =CHCHO | MeOH | 1.6×10^{3} *1.1× 10 ³ | 89 | -10 | Od-15 | S = MB. k derived using $k_d = 1.4 \times 10^5$ (*1.0 × 10 ⁵) s ⁻¹ [1.3]. | Carm.73F479 |
| 2.23 | 1-cyclopropyl-2-methylpropene | (Me) ₂ CO | $k_{\rm r}=8.6\times10^{\rm 5}$ | | rt | Ad-17 A'd | S = Eos, A' = (dicyclo- propylmethylidene)- cyclobutane. Measured $(k_r/k_r^{A'}) = 0.66$. k_r derived using $k_r^{A'} =$ $1.3 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [2.19.4]. | Rous78F430 |
| 2.24 | 1,1-dicyclo- propyl-propene | (Me) ₂ CO | $k_{\rm r}=6.5\times10^5$ | | rt | Ad-17 A'd | | Rous78F430 |
| 2.25 | 1,1-dicyclo- propyl-2-methyl- propene | (Me)₂CO | $k_r = 8.5 \times 10^5$ | | rt | Ad-17 A'd | S = Eos, A' = (dicyclo- propylmethylidene)- cyclobutane. Measured (k_r/k_r^A) = 0.65. k_r derived using $k_r^{A'}$ = $1.3 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [2.19.4]. | Rous78F430 |
| 2.26 | 1,1-dicyclo- propyl-2-methyl- propene- d_6 | For more Me ₂ CO | relative rates see $k_{\rm r} = 8.5 \times 10^{\rm s}$ | 2.26. | rt | ? | S = Eos, A' = 1,1-di- cyclopropyl-2-methyl- propene. Measured $(k_r/k_r^{A'}) = 1.0. k_r$ derived using $k_r^{A'} =$ $8.5 \times 10^5 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [2.25]. $(k_r/k_r^{A'})$ measured as a product isotope effect. | Rous78F430 |
| 2.27 | (1-cyclopropylethylidene)cyclobutane | (Me) ₂ CO | $k_{\rm r}=9.1\times10^{\rm 5}$ | | rt | Ad-17 A'd | S = Eos, A' = (dicyclopropylmethylidene)-cyclobutane. Measured $(k_r/k_r^A) = 0.70$. k_r derived using $k_r^{A'} = 1.3 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [2.19.4]. | Rous78F430 |
| 2.28 | 2,3-dimethyl-1- butene $(CH_3)_2CHC(CH_3)=$ | MeOH =CH ₂ | $k_{\rm r}=7.8\times10^3$ | | 15 | Ad-17 A'd | S = MB, A' = cyclohexene Measured $(k_r/k_r^{A'})$ = 1.7 ± 0.4. k_r derived using $k_r^{A'}$ = 4.6 × 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. Su | ubstrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|-------------------------------------|--|---------------------------------------|----------|--------------|--|-------------|
| 2.29 | cis-2-butene CH ₃ CH=CHCH ₃ | CCl ₄ /MeC (96:4) v:v | OH $(5.5 \pm 2.5) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F162 |
| 2.30 | trans-2-butene CH ₃ CH = CHCH ₃ | | OH $(1.5 \pm 0.5) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F162 |
| | 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 ₃ CH=CHCHO | МеОН | 2.2×10^3 *1.5 × 10 ³ | 65 | -10 | Od-15 | S = MB. k derived using $k_d = 1.4 \times 10^5$ (*1.0 × 10 ⁵) s ⁻¹ [1.3.6]. | Carm.73F479 |
| | 2-methyl-2-butene $CH_3CH = C(CH_3)_2$ | MeOH(?) | 1.8×10^{6} | 5.5×10^{-2} | rt | ? | Method not given. $k \text{ derived using } k_d = 1.0 \times 10^5 \text{ s}^{-1} [1.3.6].$ | Goll62F005 |
| 2.33.1 | | МеОН | 1.7×10^{5} | 6.0 × 10 ⁻¹ | 20 | Od-15 | | Koch68F288 |
| 2.33.2 | | МеОН | 1.8×10^6 | 5.5 × 10 ⁻² | 20 | Od-15 | S = tetrachloroeosin. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. E_a = 6.3 kJ mol ⁻¹ . | Koch68F288 |
| 2.33.3 | | МеОН | 1.7×10^6 | 6.0×10^{-2} | 20 | Od-15 | S = tetrachloro- fluorescein. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. E_a = 6.7 kJ mol ⁻¹ . | Koch68F288 |
| 2.33.4 | | МеОН | 1.0×10^{6} | 1.0×10^{-1} | 20 | Od-15 | $E_a = 0.00$ Me have $E_a = 0$ | Koch68F288 |
| 2.33.5 | | МеОН | 3.3×10^6 | 3.0×10^{-2} | 20 | Od-15 | S = binaphthalene- thiophene. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. E_a = 5.9 kJ mol ⁻¹ . | Koch68F288 |
| 2.33.6 | | МеОН | 1.1×10^{6} | 1.0×10^{-1} | ? | ? | Unpublished data. Method not given. k derived using $k_d = 1.1 \times 10^5 \text{ s}^{-1} [1.3.4]$. | 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [3.63.3] and k_d = 1.67 × 10 ⁴ s ⁻¹ [1.5]. | Monr78A005 |
| 2.33.8 | | EtOH | 4.8 × 10 ⁴ | 1.65 | rt | Ad-15 | | Brki76F041 |
| 2.33.9 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=7.3\times10^5$ | | 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [A3.2]. | Higg68F292 |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t ∕°C | Method | Comments | Ref. |
|---|------------------------------|--|--|---------------------|-------------------------------|--|----------------|
| 2.33.10 | MeOH /t-BuOH (1:1) v:v | $k_{\rm r} = 8.6 \times 10^{\rm s}$ | | 25 | Pa-17 P'a | $^{1}O_{2}$ * from H ₂ O 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 | Higg68F29 |
| 2.33.11 | MeOH /t-BuOF (1:1) v:v | $k_{\rm r}=1.4\times10^6$ | | rt | Ad-17 A'd | s ⁻¹ [A3.2]. S = RB, A' = TME. Measured $(k_r^{A'}/k_r) = 22$. k_r derived using $k_r^{A'} =$ *3.0 × 10 ⁷ dm ³ | Higg68F29 |
| 2.33.12 | MeOH /t-BuOF (1:1) v:v | $k_{\rm r}=2.0\times10^6$ | | rt | Ad-17 A'd | mol ⁻¹ s ⁻¹ [A3.2]. ¹ O ₂ * from H ₂ O 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 | Higg68F29 |
| 2.33.13 | MeOH /t-BuOF (1:1) v:v | | , | rt | Ad-17 A'd | s ⁻¹ [A3.2]. ¹ O ₂ * from H ₂ O ₂ /Ca(OCl) ₂ , A' = TME. Measured $(k_r^{A'}/k_r) = 23. k_r$ derived using $k_r^{A'} = *3.0 \times 10^7$ dm ³ mol ⁻¹ s ⁻¹ [A3.2]. | Higg68F29 |
| | For more | relative rates see | 2.40.27, 2.40.28, 2.42 2.52.8, 2.56.14, 2.56. | 2.3, 2.4 15, 3.1 | 2.4, 2.43.1, 2 13 13 2 | 2.43.2, 2.52.7, | |
| 2.34 trans-2-cyclo- propyl-2-butene | (Me)₂CO | $k_{\rm r}=6.9\times10^{\rm s}$ | | rt | | S = Eos, A' = (dicyclo- propylmethylidene)- cyclobutane. Measured (k_r/k_r^A) = 0.53. k_r derived using $k_r^{A'}$ = | Rous78F43 |
| CH3 H | | | | | | $1.3 \times 10^6 \mathrm{dm^3 mol^{-1} s^{-1}}$ | |
| 2.35 2,3-dimethyl- 2-butene (TME) $(CH_3)_2C=C(CH_3)_2$ | | 3.3×10^7 | 3.0×10^{-3} | rt | ? | [2.19.4]. Method not given. k derived using $k_d = *1.0 \times 10^5$ | Goll62F005 |
| 2.35.1 | МеОН | 1.6×10^7 | 6.2×10^{-3} | 20 | Od-15 | s^{-1} [1.3.6]. S = RB. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. $E_a =$ | Koch68F288 |
| 2.35.2 | МеОН | 2.2×10^7 | $(4.6 \pm 0.5) \times 10^{-3}$ | 23 | A'd-16 | 2.1 kJ mol ⁻¹ . S = MB, A' = DPBF, k derived using $k_d =$ | Youn71F39 |
| 2.35.3 | MeOH | $(4.0 \pm 1.0) \times 10^7$ | | rt | A'd-5 | *1.0 \times 10 ⁵ s ⁻¹ [1.3.6]. S = MB, A' = DPBF, | Merk.71M32 |
| 2.35.4 | CHCl ₃ | $(5.8 \pm 0.9) \times 10^7$ | | rt | A'd-33 | ruby laser (694 nm). $S = A' = Rub. k$ | Monr78A005 |
| | | , | | | | derived using $k_A = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3] and $k_d = 1.67 \times 10^4 \text{ s}^{-1}$ [1.5]. | |
| 2.35.5 | EtOH | 1.6 × 10 ⁷ *3.2 × 10 ⁷ | · | rt | Od-23 | S = RB, A' = hexa- methylenedithiocarbamate. Measured $k/(k_d + k_A \{A'\}) = 270$ at $[A'] = 2.8 \times 10^{-4}$ mol dm ⁻³ . k derived using $k_{A'} = 1.5 \times 10^8$ dm ³ mol ⁻¹ s ⁻¹ [11.42] and $k_d = 1.0 \times 10^4$ (*7.9 × 10 ⁴) s ⁻¹ [1.10.3]. | Yama72F11 = |

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

| No. Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t 1 /°C | Method | Comments | Ref. |
|-------------------|---|--|--|-------------------------|---------------------------|--|-------------|
| 2.35.6 | EtOH | 1.4 × 10 ⁵ | 5.6 × 10 ⁻¹ | rt | Ad-15 | S = MB. k derived using $k_d = *7.9 \times 10^4$ s ⁻¹ [1.10.3]. Reported values are suspect since r_{ox} depends on $[O_2]$ and β value was determined | Brki76F041 |
| 2.35.7 | (Me) ₂ CO | 5.4×10^{7} $*4.3 \times 10^{7}$ | $(7.2 \pm 0.2) \times 10^{-4}$ | 15 | A'd-16 | from nonlinear data plots. $S = RB$, $A' = DPBF$. k derived using $k_d = 3.8 \times 10^4$ (*3.1 \times 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 $k_d =$ | Youn71F398 |
| 2.35.9 | t-BuOH | 1.0×10^7 | $(2.9 \pm 0.3) \times 10^{-3}$ | 23 | A'd-16 | $5.2 \times 10^4 \text{ s}^{-1}$ [1.24]. S = MB, A' = DPBF. $k \text{ derived using } k_d =$ | Youn71F398 |
| 2.35.10 | C,H,N | 1.6×10^7 | | ~10 | A'd-20 | $3.0 \times 10^4 \text{s}^{-1} [1.25].$ S = A' = DPBF. Measured $(k/k_{A'}) =$ $2.6 \times 10^{-2}. k \text{derived}$ using $k_{A'} = *6.3 \times 10^8$ dm³ mol ⁻¹ s ⁻¹ [A3.17]. | Wils66F014 |
| 2.35.11 | C₅H₅N | 4.5×10^{7} | 1.3×10^{-3} | 12 | Pa-20 | S = thionine,MB,DMA A' = DMA. k derived using $k_d = 5.9 \times 10^4$ s ⁻¹ [1.29.1]. β is the | Kram.73F202 |
| 2.35.12 | C_6H_6 | 5.2 × 10 ⁷ | 7.7 × 10 ⁻⁴ | 25 | A'd-23 | same for all 3 S. S = A' = DMA. k derived using $\beta_{A'} = 3.0 \times 10^{-4}$ mol dm ⁻³ [3.53.21] and $k_d = *4.0 \times 10^4$ 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. $kderived using \beta_{A'} = 7.1 \times 10^{-4} mol dm-3 [3.61.2] and k_d = *4.0 \times 10^4 s-1 [1.32.9].$ | 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 $\beta_{A'} = 1.7 \times 10^{-3}$ mol dm ⁻³ [3.62.4] and $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Alga.70E079 |
| 2.35.15 | C ₆ H ₆ | 5.6×10^7 | 7.14 × 10 ⁻⁴ | 25 | A'd-23 | S = A' = Rub. k derived using $\beta_{A'} = 3.0 \times 10^{-4} \text{ mol}$ $dm^3 [3.63.15] \text{ and } k_d = *4.0 \times 10^4 \text{ s}^{-1} [1.32.9].$ | Alga.70E079 |
| 2.35.16 | C ₆ H ₅ CH ₃ | 4.2×10^7 | | rt | A'd-5 | S = Naph, A' = DPBF. Sensitizer excited with pulsed electron beam (10 MeV). | Gorm78E26 |
| 2.35.17 | MeOH /t-BuOH (1:1) v:v | , , | $(2.3 \pm 0.3) \times 10^{-3}$ | rt | A'd-16 | S = RB, A' = DPBF. k estimated using $k_d = 7.9 \times 10^4 \text{ s}^{-1}$ (calc). | Youn71F398 |
| | For more r | elative rates see | 2.3.2, 2.12.3, 2.33.9–1 2.91.5–6, 3.35, 3.35.1 3.56.5, 3.63.10–11, 4. 6.21, 6.21.1–8, 7.1, 7. | , 3.43, 3. 16, 4.16. | .43.1, 3.53 1, 5.29.15 | .15, 3.53.26, –17, 5.36.89, | |

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

| No. S | ubstrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|--|--|---------------------------------------|----------|--------------|---|------------|
| 2.36 | 2-cyclopropyl- 3-methyl-2-butene | | $k_{\rm r}=9.9\times10^5$ | | rt | Ad-17 A'd | S = Eos, A' = (dicyclo- propylmethylidene)- cyclobutane. Measured | Rous78F43 |
| | \nearrow | | | | | | $(k_r/k_r^{A'}) = 0.76. k_r$ derived using $k_r^{A'} =$ | |
| | CH3/2C=C | | | | | | $1.3 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [2.19.4]. | |
| .37 | 1-pentene $CH_3(CH_2)_2CH = CH_3(CH_2)_2CH = CH_2(CH_2)_2CH = CH_2(CH_2)$ | CCl ₄ /Me0 I ₂ (96:4) v:v | OH $(1.0 \pm 0.4) \times 10^3$ | | rt | A'd-8 | S = MB, $A' = DPBF$, ruby laser (694 nm). | Bort77F1 |
| .38 | cis-2-pentene CH ₃ CH ₂ CH = CHC | | OH $(4.0 \pm 1.5) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F1 |
| .39 | trans-2-pentene CH ₃ CH ₂ CH = CHC | | OH $(2.0 \pm 0.8) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F1 |
| .40 | 2-methyl-2- pentene (2M2P) CH ₃ CH ₂ CH=C(Cl | | 5.6×10^5 | 1.8×10^{-1} | rt | ? | Method not given. k derived using $k_d =$ | Goll62F00 |
| .40.1 | | MeOH | 7.7×10^5 | 1.3×10^{-1} | 20 | Od-15 | *1.0 \times 10 ⁵ s ⁻¹ [1.3.6]. S = RB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_s =$ | Koch68F28 |
| 40.2 | | МеОН | 6.25×10^{5} | $(1.6 \pm 0.3) \times 10^{-1}$ | 25 | Pa-15 | 8.4 kJ mol ⁻¹ . S = RB. k derived using $k_d = *1.0 \times 10^5$ | Foot.71F3 |
| 40.3 | | МеОН | 7.7×10^{5} | $(1.3 \pm 0.1) \times 10^{-1}$ | 25 | Pa-15 | s ⁻¹ [1.3.6]. S = chlorophyll-b. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. | Foot.71F3 |
| 40.4 | | MeOH | 5.0 × 10 ⁵ | $(2.0 \pm 0.8) \times 10^{-1}$ | 25 | Pa-15 | S = chlorophyll-a. k derived using $k_d = 1.0 \times 10^5 \text{ s}^{-1} [1.3.6]$. | Foot.71F3 |
| 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 × 10 ⁵ s ⁻¹ [1.3.6]. | Youn71F |
| 40.6 | | МеОН | 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.71F5 |
| 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 × 10 ⁵ s ⁻¹ [1.3.6]. | Chai.76F90 |
| 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [3.63.3] and k_d = 1.67 × 10 ⁴ s ⁻¹ [1.5]. | Monr78A0 |
| .40.9 | | CS ₂ | 6.25×10^4 | $(8.0 \pm 1.0) \times 10^{-2}$ | 0 | Pa-15 | $S = ZnTPP$. k derived using $k_d = 5.0 \times 10^3 \text{ s}^{-1} [1.9]$. | Foot.71F3 |
| 40.10 | | CH ₃ CN | 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.71F5 |
| .40.11 | | CH ₃ CN | 1.4×10^6 | 1.8×10^{-2} | rt | Od-15 | S = RB. k derived using $k_d =$ *2.55 × 10 ⁴ s ⁻¹ [1.17.2]. | Smit75F1 |
| .40.12 | | C ₂ H ₅ I | 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.71F3 |

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

| No. Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|-----------------------------------|--|---------------------------------------|----------|--------------|---|-------------|
| 2.40.13 | (Me) ₂ SO | 7.4×10^{5} (est) | $(7.0 \pm 1.0) \times 10^{-2}$ | 25 | Pa-15 | S = RB. k estimated using $k_d = 5.2 \times 10^4 \text{ s}^{-1}$ [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 = 5.2×10^4 s ⁻¹ [$I(a)$. I]. | 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) ₂ CO | 3.9×10^{5} | $(8.0 \pm 1.0) \times 10^{-2}$ | 25 | Pa-15 | S = RB. k derived using $k_d = *3.1 \times 10^4 \text{ s}^{-1} [1.22.2].$ | 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 $k_d = 3.0 \times 10^4 \text{ s}^{-1}$ [1.25]. | Youn71F39 |
| 2.40.18 | C ₅ H ₅ N | 1.2×10^{6} | $(5.0 \pm 1.0) \times 10^{-2}$ | 25 | Pa-15 | S = RB. k derived using $k_d = 5.9 \times 10^4 \text{s}^{-1} [1.29.1].$ | Foot.71F356 |
| 2.40.19 | C ₅ H ₅ N | 1.4×10^{6} | 4.3×10^{-2} | rt | Od-15 | | Smit75F166 |
| 2.40.20 | C ₆ H ₁₁ OH | 9.0×10^{5} | $(7.0 \pm 1.0) \times 10^{-2}$ | 25 | Pa-15 | S = RB. k derived using $k_d = 6.3 \times 10^4 \text{ s}^{-1} [1.31].$ | Foot.71F356 |
| 2.40.21 | C ₆ H ₆ | 1.7×10^{5} | $(2.3 \pm 1.2) \times 10^{-1}$ | rt | Pa-15 | S = ZnTPP. k derived using $k_d = *4.0 \times 10^4$ 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 $k_d = *4.0 \times 10^4$ 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]. | Smit75F166 |
| 2.40.24 | C₀H₅Br | 2.6×10^{5} | $(5.0 \pm 3.0) \times 10^{-2}$ | 25 | Pa-15 | S = ZnTPP. k derived using $k_d = 1.3 \times 10^4 \text{s}^{-1} [1.34]$. | 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 ₆ H ₅ CH 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 | 2 2 | Foot.71F356 |
| 2.40.27 | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=1.1\times10^6$ | | 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]. | Higg68F292 |
| 2.40.28 | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=1.2\times10^6$ | | 25 | Pa–17 P'a | ${}^{1}O_{2}$ * from ${}^{1}O_{2}$ /NaOCl, ${}^{1}O_{2}$ * from ${}^{1}O_{2}$ /NaOCl, ${}^{2}O_{2}$ -methyl-2-butene. Measured $(k_{r}^{A'}/k_{r}) = 1.28$. k_{r} derived using $k_{r}^{A'} = *1.5 \times 10^{6} \text{ dm}^{3}$ ${}^{2}O_{2}$ mol ${}^{-1}$ s ${}^{-1}$ [$A3.1$]. | Higg68F292 |
| 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 $k_d = 7.9 \times 10^4 \text{ s}^{-1} \text{ (calc)}.$ | Youn71F39 |

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

| (4:1) v.v | No. Substrate (A) | Solvent k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t Method | Comments | Ref. |
|---|---------------------------------|--|---------------------------------------|-----------|---|-------------|
| 2.45, 2.45, 1, 2.46, 2.46, 1, 2.56, 12-13, 2.119, 2.121, 2.123, 1.243, 1.246, 2.461, 2.56, 12-13, 2.119, 2.121, 2.123, 1.242.126, 1.2166, 1.2130.9, 2.132, 4.7.2, 4.7.8-9, 4.9.1, 4.12.4. 2.41 2-methyl-2-pent- MeOH | 2.40.30 | | $(5.0 \pm 0.5) \times 10^{-2}$ | rt Pa-15 | using $k_d =$ | Foot.71F356 |
| cne-4-ol CH,CH(OH)CH=C(CH ₁); cts-3-methyl-2- CHCl ₃ pentene CH ₃ CH ₂ C(CH ₃)=CHCH ₃ 2.42.1 MeOH k _r = 8.3 × 10 ³ /r-BuOH (1:1) v:v 2.42.2 MeOH k _r = 1.2 × 10 ⁶ /r-BuOH (1:1) v:v 2.42.3 MeOH k _r = 8.3 × 10 ³ /r-BuOH (1:1) v:v 2.42.4 MeOH k _r = 8.3 × 10 ³ /r-BuOH (1:1) v:v 2.42.5 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.42.6 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.42.7 MeOH k _r = 6.0 × 10 ³ /r-BuOH (1:1) v:v 2.42.8 MeOH k _r = 6.0 × 10 ³ /r-BuOH (1:1) v:v 2.42.9 MeOH k _r = 8.3 × 10 ³ /r-BuOH (1:1) v:v 2.42.1 MeOH k _r = 8.3 × 10 ³ /r-BuOH (1:1) v:v 2.42.2 MeOH k _r = 8.3 × 10 ³ /r-BuOH (1:1) v:v 2.42.3 MeOH k _r = 8.3 × 10 ³ /r-BuOH (1:1) v:v 2.42.4 MeOH k _r = 8.3 × 10 ³ /r-BuOH (1:1) v:v 2.42.5 EIOH 1.3 × 10 ⁶ /r-BuOH (1:1) v:v 2.43.1 MeOH k _r = 6.0 × 10 ³ /r-PrOH (est) (1:1) v:v 2.44.3 Imans-3-methyl-2- CHCl ₃ /r-PrOH (est) (1:1) v:v 2.45.3 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.46.4 Imans-3-methyl-2- CHCl ₃ (1:1) v:v 2.47.4 Imans-3-methyl-2- CHCl ₃ (1:1) v:v 2.48.5 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.49.6 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.40.7 Imans-3-methyl-2- CHCl ₃ (1:1) v:v 2.41.1 MeOH k _r = 1.2 × 10 ⁶ /r-BuOH (1:1) v:v 2.42.5 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.43.1 MeOH k _r = 1.2 × 10 ⁶ /r-BuOH (1:1) v:v 2.44.5 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.45 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.46 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.47 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.48 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.49 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.40 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.41 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.42 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.43 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.44 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.45 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.46 EIOH 1.3 × 10 ⁶ (1:1) v:v 2.47 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.48 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.49 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.40 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.41 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.42 Imans-3-methyl-2- Chlcl ₃ (1:1) v:v 2.43 Imans-3 Imanship imanship imansh | | For more relative rates see | 2.126, 2.126.1, 2.136 | | .119, 2.121, 2.123, | |
| 2.42 cis 3 methyl-2 CHCl ₃ $(2.0 \pm 0.3) \times 10^6$ rt A' d-33 $S = A' = Rub, k$ derived using $k_A' = 5.3 \times 10^3$ and $k_a = 1.67 \times 10^6 \times 10^5 \times 10^5$ rt Ad -17 $S = RB, A' = TME$. Hig A' d Measured $(k_1^A/k_1) = 1.2 \times 10^6$ $(1:1) v \cdot v$ Ad -17 $S = RB, A' = TME$. Hig A' d Measured $(k_1^A/k_2) = 1.8 \times 10^3 \times 10^3$ | ene-4-ol | | | | k derived using $k_{\rm d} =$ | Chai.76F909 |
| 2.42.1 MeOH $k_r = 8.3 \times 10^3$ //-BuOH (1:1) v:v 2.42.2 MeOH $k_r = 1.2 \times 10^6$ //-BuOH (1:1) v:v 2.42.3 MeOH $k_r = 1.2 \times 10^6$ //-BuOH (1:1) v:v 2.42.3 MeOH $k_r = 8.3 \times 10^5$ //-BuOH (1:1) v:v 2.42.4 MeOH $k_r = 8.3 \times 10^5$ //-BuOH (1:1) v:v 2.42.5 MeOH $k_r = 8.3 \times 10^5$ //-BuOH (1:1) v:v 2.42.6 MeOH $k_r = 8.3 \times 10^5$ //-BuOH (1:1) v:v 2.42.7 MeOH $k_r = 8.3 \times 10^5$ //-BuOH (1:1) v:v 2.42.8 MeOH $k_r = 8.3 \times 10^5$ //-BuOH (1:1) v:v 2.42.9 The second of the se | 2.42 cis-3-methyl-2- pentene | $CHCl_3$ (2.0 ± 0.3) × | 106 | 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] | Monr78A005 |
| 2.42.2 MeOH $k_r = 1.2 \times 10^6$ rt Ad-17 1 O,* from H,O,/NaOCl, Hig (l:1) v:v (R/ 1 k, D = 1.2 × 10 6 (R/ 1 k, D = 2.5 k, derived using k_r = 3.0 × 10 7 dm morl s -1 [A3.2]. rt Ad-17 1 S = RB, A' = 2-methyl- A'd 2-butene. Measured (k, 1 /k, D = 1.8 k, derived using k_r = 1.5 × 10 6 dm morl s -1 [A3.1]. rt Ad-17 1 O,* from H,O,/NaOCl, Hig (k, 1 /k, D = 1.8 k, derived using k_r = 1.5 × 10 6 dm morl s -1 [A3.1]. rt Ad-17 1 O,* from H,O,/NaOCl, Hig (k, 1 /k, D = 1.8 k, derived using k_r = 1.5 × 10 6 dm morl s -1 [A3.1]. rt Ad-17 1 O,* from H,O,/NaOCl, Hig (k, 1 /k, D = 1.8 k, derived using k_r = 1.5 × 10 6 dm morl s -1 [A3.1]. rt Ad-17 1 O,* from H,O,/NaOCl, Hig (k, 1 /k, D = 1.8 k, derived using k_r = 1.5 × 10 6 dm morl s -1 [A3.1]. rt Ad-17 1 O,* from H,O,/NaOCl, Hig (k, 1 /k, D = 1.8 k, derived using k_r = 1.5 × 10 6 dm morl s -1 [A3.1]. rt Ad-17 1 O,* from H,O,/NaOCl, Hig (k, 1 /k, D = 1.5 × 10 6 dm morl s -1 [A3.1]. rt Ad-18 S = RB, A' = 2-methyl-2-butene. Measured (k, 1 /k, D = 1.2 k, derived using k_r = 1.67 × 10 6 s -1 [A3.1]. rt Ad-18 S = RB, A' = 2-methyl-2-butene. Measured (k, 1 /k, D = 1.2 k, derived using k_r = 1.67 × 10 6 s -1 [A3.1]. Hig (k, 1 /k) = 1.2 k, derived using k_r = 1.5 × 10 6 dm morl s -1 [A3.1]. | 2.42.1 | /t-BuOH |)5 | | S = RB, A' = TME. Measured $(k_r^{A'}/k_r)$ = 36. k_r derived using $k_r^{A'}$ = *3.0 × 10 ⁷ dm ³ | Higg68F292 |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$ | | /t-BuOH | 96 | | $^{1}O_{2}$ * from H ₂ O 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 | Higg68F292 |
| 2.42.4 MeOH $k_r = 6.0 \times 10^5$ rt Ad-17 1O_2* from $H_2O_2/Ca(OCl)_2$, Hig A'= BuOH (1:1) v:v Ad-17 1O_2* from $H_2O_2/Ca(OCl)_2$, Hig A'= 2-methyl-2-butene. Measured $(k_r^{A'}/k_r) = 2.5$. k_r derived using $k_r^{A'} = *1.5 \times 10^6$ dm³ mol ⁻¹ s ⁻¹ [A3.1]. 2.42.5 EtOH 1.3 × 10 ⁶ 5.0 × 10 ⁻² 19 Od-14 S = RB, A' = DMF. k Sch A'= PrOH (est) (1:1) v:v estimated using $k_d = 6.7 \times 10^6$ s ⁻¹ (calc). 2.43 $trans$ -3-methyl-2- CHCl ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.44.3 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.45.4 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.46.3 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.47 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.48 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.49 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.40 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.40 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.41 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.42 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.43 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A . 2.43 $trans$ -3-methyl-2- CHCH ₃ (1.5 ± 0.3) × 10 ⁶ rt A'd-33 S = A' = Rub. k derived using k_A = 1.5 × 10 ⁶ dm³ mol ⁻¹ s ⁻¹ [1.5]. | 2.42.3 | /t-BuOH | | | 2-butene. Measured $(k_r^{A'}/k_r) = 1.8. k_r$ derived using $k_r^{A'} = *1.5 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ | Higg68F292 |
| 2.42.5 EtOH 1.3×10^6 5.0×10^{-2} 19 Od-14 S = RB, A' = DMF. k Sch /i-PrOH (est) 27 estimated using $k_d = 6.7 \times 10^4 \text{ s}^{-1}$ (calc). 2.43 $trans$ -3-methyl-2- CHCl ₃ $(1.5 \pm 0.3) \times 10^6$ rt A'd-33 S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3] and $k_d = 1.67 \times 10^4 \text{ s}^{-1}$ [1.5]. 2.43.1 MeOH $k_r = 1.2 \times 10^6$ rt Ad-17 S = RB, A' = 2-methyl- Hig A'd 2-butene. Measured $(k_r / k_r) = 1.2 \times k_r$ derived using $k_r = 1.5 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [43.1]. | 2.42.4 | /t-BuOH | y. | | $^{1}O_{2}*$ from $H_{2}O_{2}/Ca(OCl)_{2}$, A' = 2-methyl-2-butene. Measured $(k_{r}^{A'}/k_{r}) = 2.5$. k_{r} derived using $k_{r}^{A'} =$ $*1.5 \times 10^{6} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ | Higg68F292 |
| 2.43 $trans-3$ -methyl-2- 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 dm³ mol ⁻¹ s ⁻¹ [3.63.3] and k_d = 1.67×10^4 s ⁻¹ [1.5]. rt Ad-17 S = RB, A' = 2-methyl- Hig A'd 2-butene. Measured $(k_r^{A'}/k_r) = 1.2 \times k_r$ derived using $k_r^{A'}$ = *1.5 × 10 ⁶ dm³ mol ⁻¹ s ⁻¹ [A3.1]. | | /i-PrOH (est) (1:1) v:v | 5.0×10^{-2} | | S = RB, A' = DMF. k estimated using | Schu78F464 |
| 2.43.1 MeOH $k_r = 1.2 \times 10^6$ rt Ad-17 S = RB, A' = 2-methyl- Hig /t-BuOH (1:1) v:v Ad 2-butene. Measured $(k_r^{\Lambda'}/k_r) = 1.2. k_r$ derived using $k_r^{\Lambda'} = *1.5 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [A3.1]. | pentene | | 106 | rt A'd-33 | S = A' = Rub. k derived using $k_{A'}$ = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3] and k_d = | Monr78A005 |
| | | /t-BuOH | , | | 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 | Higg68F292 |
| /t-BuOH (1:1) v:v A'd 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 | 2.43.2 | /t-BuOH | 9 6 | | ${}^{1}O_{2}$ * from H ₂ O ₂ /Ca(OCl) ₂ , A' = 2-methyl-2-butene. Measured $(k_{r}^{A'}/k_{r}) = 1.4$. k_{r} derived using $k_{r}^{A'} =$ | Higg68F29 |

CHEMICAL KINETICS OF SINGLET OXYGEN IN SOLUTION

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

| No. S | Substrate (A) | Solvent | /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|---|---|---------------------------------------|----------|--------------|--|------------|
| 2.43.3 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=4.4\times10^6$ | | rt | Ad-17 A'd | S = RB, A' = 1-methyl-cyclohexene. 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]. | Higg68F29 |
| 2.43.4 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=1.4\times10^6$ | | rt | Ad-17 A'd | $^{1}O_{2}$ * from $H_{2}O_{2}$ /Ca(OCI) 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]. | Higg68F29 |
| 2.43.5 | | EtOH / <i>i</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 $k_d = 6.7 \times 10^4 \text{ s}^{-1}$ (calc). | Schu78F46 |
| 2.44 | 3-methyl- 2-pentene (cis,trans mix) | C ₆ H ₅ Cl | 1.0×10^6 (est) | 1.6×10^{-2} | 25 | Ad-15 | | Carl74F341 |
| 2.45 | cis-4-methyl- 2-pentene $(CH_3)_2CHCH = CH$ | MeOH /t~BuOH (1:1) v:v CH ₃ . | $k_{\rm r}=1.1\times10^4$ | | 30 | Pa-17 P'a | S = RB, A' = 2M2P. Measured $(k_t/k_r^{A'})$ = 1.4 × 10 ⁻² . k_r derived using $k_r^{A'}$ = *8.1 × 10 ⁵ dm³ mol ⁻¹ s ⁻¹ [A3.3]. | Higg68F29 |
| 2.45.1 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=8.9\times10^3$ | | 3–4 | Pa-17 P'a | $^{1}O_{2}$ * from $H_{2}O_{2}/NaOCl$, A' = 2M2P. Measured $(k_{r}/k_{r}^{A}) = 1.1 \times 10^{-2}$. k_{r} derived using $k_{r}^{A'} =$ *8.1 × 10 ⁵ dm ³ mol ⁻¹ s ⁻¹ [A3.3]. | Higg68F29 |
| 2.45.2 | | MeOH /t-BuOH (1:1) v:v | , , | 8.0 ± 0.8 | rt | A'd-16 | S = RB, A' = DPBF. k estimated using k_d = $7.9 \times 10^4 \text{ s}^{-1}$ (calc). | Youn71F39 |
| 2.46 | trans-4-methyl- 2-pentene $(CH_3)_2CHCH = CH^{-1}$ | MeOH /t-BuOH (1:1) v:v | elative rates see $k_{\rm r} = 2.0 \times 10^3$ | 2.54.2. | 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]. | Higg68F29 |
| 2.46.1 | | MeOH /t~BuOH (1:1) v:v | $k_{\rm r} = 1.6 \times 10^3$ | | 3–4 | Pa-17 P'a | In mol s [A3.3]. $^{1}O_{2}$ * from $H_{2}O_{2}/NaOCl$, A' = 2M2P. Measured $(k_{r}/k_{r}^{A}) = 2.0 \times 10^{-3}$. k_{r} derived using $k_{r}^{A} =$ *8.1 × 10 ⁵ dm ³ mol ⁻¹ s ⁻¹ [A3.3]. | Higg68F292 |
| 2.47 | 2,4-dimethyl- 2-pentene (CH ₃) ₂ CHCH=C(C | MeOH(?) | 7.7×10^4 | 1.3 | rt | ? | Method not given. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Goll62F005 |
| 2.47.1 | , ,,, | | $(4.3 \pm 0.7) \times 10^5$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ $[3.63.3] \text{ and } k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5].$ | Monr78A00 |
| 2.48 | 2,3,4-trimethyl- 2-pentene (CH ₃) ₂ CHC(CH ₃)= | , | $(3.9 \pm 0.6) \times 10^7$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ $\{3.63.3\} \text{ and } k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5].$ | Monr78A00 |

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

| No. | Substrate (A) | Solvent | /dm³ mol-1 s-1 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|-------------------------------|---|---------------------------------------|----------|--------------|---|-------------|
| 2.49 | 2,4,4-trimethyl- 2-pentene (CH ₃) ₃ CCH=CH(C | | 2.4×10^4 | 4.2 | rt | ? | Method not given. k derived using $k_d =$ | Goll62F005 |
| 2.50 | cyclopentene | MeOH | $k_{\rm r}=7.0\times10^4$ | | 15 | Ad-17 A'd | *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. 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 | Kope.65F02 |
| | | For more | relative rates see | 2.53. | | | $dm^3 mol^{-1} s^{-1} [2.59].$ | |
| 2.51 | 3,5-dioxacyclo- pentene | (Me) ₂ CO | 1.2×10^7 *9.5 × 10 ⁶ | $(3.28 \pm .04) \times 10^{-3}$ | 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-methyl-cyclopentene | МеОН | $k_{\rm r}=2.1\times10^5$ | | 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.65F02 |
| 2.52.1 | | CHCl ₃ | $(2.7 \pm 0.4) \times 10^6$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'}$ = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3] and k_d = $1.67 \times 10^4 \text{ s}^{-1}$ [1.5]. | Monr78A00 |
| 2.52.2 | | CH ₃ CN | $k_r = 1.5 \times 10^6$ | | rt | ? | S = MB, A' = 1-methyl- cyclohexene. 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]. | Jeff73F66 |
| 2.52.3 | | C ₆ H ₆ | 2.3×10^6 | 1.75×10^{-2} | 25 | A'd-23 | S = A' = DMA. k derived using $\beta_{A'} = 3.0 \times 10^{-4}$ mol dm ⁻³ [3.53.21] and $k_d = *4.0 \times 10^4$ s ⁻¹ | Alga.70E079 |
| 2.52.4 | | C ₆ H ₆ | 2.5 × 10 ⁶ | 1.6×10^{-2} | 25 | A'd-23 | [1.32.9]. S = A' = DMBA. $kderived using \beta_{A'} = 7.1 \times 10^{-4} moldm^{-3} [3.61.2] and k_d = 10^{-4}$ | Alga.70E079 |
| 2.52.5 | • | C ₆ H ₆ | 2.3×10^6 | 1.75×10^{-2} | 25 | A'd-23 | *4.0 × 10 ⁴ s ⁻¹ [1.32.9]. S = A' = Tetr. k derived using $\beta_{A'}$ = 1.7 × 10 ⁻³ mol dm ⁻³ [3.62.4] and k _d = | Alga70E079 |
| 2.52.6 | | C ₆ H ₆ | 2.2 × 10 ⁶ | 1.8×10^{-2} | 25 | A'd-23 | *4.0 \times 10 ⁴ s ⁻¹ [1.32.9]. S = A' = Rub. k derived using $\beta_{A'}$ = 3.0 \times 10 ⁻⁴ mol dm ⁻³ [3.63.15] and k_d = *4.0 \times 10 ⁴ s ⁻¹ [1.32.9]. | Alga.70E079 |

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

| No. S | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|-------------------------------|---|--|---------------------------------------|----------|---------------|---|-------------|
| 2.52.7 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=1.5\times10^6$ | | 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]. | Higg68F292 |
| 2.52.8 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=9.4\times10^{\rm 5}$ | | rt | Ad-17 A'd | | Higg68F292 |
| 2.52.9 | | ? | $k_{\rm r}=1.2\times10^6$ | | rt | ? | Experimental method unclear, $A' = 1$ -methyl-cyclohexene. Measured $(k_r/k_r^{A'}) = 6.2$. k_r derived using $k_r^{A'} = *2.0 \times 10^5$ dm ³ mol ⁻¹ s ⁻¹ [A3.5]. | Foot.71F580 |
| 2.53 | 2-hexene $CH_3(CH_2)_2CH = C$ | MeOH | elative rates see $k_{\rm r}=3.9\times10^4$ | 2.56.1–5. | 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 × 10 ⁴ dm ³ mol ⁻¹ s ⁻¹ [2.50]. | Kope.65F028 |
| 2.54 | cyclohexene | For more re MeOH(?) | elative rates see 3.8×10^3 | 2.54.1. 26 | rt | ? | Method not given. k derived using $k_d = *1.0 \times 10^5 \text{s}^{-1} [1.3.6]$. | Goll62F005 |
| 2.54.1 | | МеОН | $k_{\rm r}=4.6\times10^3$ | | 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 × 10 ⁴ | Kope.65F028 |
| 2.54.2 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=2.0\times10^3$ | | 30 | Pa-17 P'a | dm³ mol ⁻¹ s ⁻¹ [2.53]. S = RB, A' = cis-4- methyl-2-pentene. Measured $(k_r^{A'}/k_r) = 5.4$. k_r derived using $k_r^{A'} = 1.1 \times 10^4$ dm³ mol ⁻¹ s ⁻¹ [2.45]. | Higg68F292 |
| 2.54.3 | | C ₆ H ₆ /MeO (3:1) v:v | $0H 2.0 \times 10^4$ | 3.1 | 25 | Ad-15 | S = MB. k derived using $k_d = 6.25 \times 10^4$ s ⁻¹ . | Kret.78F586 |
| 2.55 | 3,6-dioxacyclo- hexene | For more re (Me) ₂ CO | elative rates see 3.6×10^5 *1.4 \times 10 ⁵ | 2.28, 2.57, 2.85. | 8 | ? | S = ?, A' = Car. Measured (k/k_A) = 1.2 × 10 ⁻⁵ . k derived using k_A = 3 × 10 ¹⁰ (*1.2 × 10 ¹⁰) dm ³ mol ⁻¹ s ⁻¹ . | Bart70F733 |
| 2.55.1 | | (Me) ₂ CO | 2.2×10^{5} *1.8 × 10 ⁵ | $(1.76 \pm .02) \times 10^{-1}$ | 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 re | elative rates see | 2.1, 2.1.2, 2.2.1, 2.3-4 | , 2.56 | .7, 2.63, 3.2 | | |

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

| No. S | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /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 $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Goll62F005 |
| 2.56.1 | | МеОН | $k_{\rm r}=2.0\times10^5$ | | 15 | Ad-17 A'd | $S = MB$, $A' = 1$ -methyl-cyclopentene. Measured $(k_r^{A'}/k_r) = 8.6 \pm 0.9$. k_r derived using $k_r^{A'} = *1.8 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [A3.4]. | Kope.65F02 |
| 2.56.2 | | МеОН | $k_{\rm r}=1.6\times10^5$ | | 15 | Ad-17 A'd | S = RB, A' = 1-methyl-cyclopentene. Measured $(k_r^{A'}/k_r) = 11.5 \pm 1.9$. k_r derived using $k_r^{A'} = *1.8 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [A3.4]. | Kope.65F02 |
| 2.56.3 | | МеОН | $k_{\rm r}=1.7\times10^5$ | | 15 | Ad-17 A'd | From Fig. 1.8 Eos, A' = 1-methylcyclopentene. Measured $(k_r^{A'}/k_r)$ = 10.8 \pm 1.4. k_r derived using $k_r^{A'}$ = *1.8 \times 106 dm³ mol ⁻¹ s ⁻¹ [43.4]. | Kope.65F02 |
| 2.56.4 | | МеОН | $k_{\rm r}=2.0\times10^5$ | | 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 dm³ mol ⁻¹ s ⁻¹ [43.4]. | Kope.65F02 |
| 2.56.5 | • | МеОН | $k_{\rm r}=1.9\times10^{5}$ | | 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 dm³ mol ⁻¹ s ⁻¹ [A3.4]. | Kope.65F02 |
| 2.56.6 | | CHCl ₃ | $(3.6 \pm 0.6) \times 10^5$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'}$ = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3] and k_d = $1.67 \times 10^4 \text{ s}^{-1}$ [1.5]. | Monr78A00 |
| 2.56.7 | | (Me) ₂ CO | $k_{\rm r} = 2.1 \times 10^{\rm s}$ *1.7 × 10 ^s | | 8 | ? | S = ?, A' = p-dioxene. Measured $(k_r/k_r^{A'})$ = 9.6×10^{-1} . k_r derived using $k_r^{A'}$ = 2.2×10^5 (*1.8 × 10 ⁵) dm ³ mol ⁻¹ | Bart70F733 |
| 2.56.8 | | C_6H_6 | 3.0×10^{5} | 1.3 × 10 ⁻¹ | 25 | A'd-23 | s ⁻¹ [2.55.1]. 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 ₆ H ₆ | 3.3×10^{5} | 1.2×10^{-1} | 25 | A'd-23 | S = A' = DMBA. k derived using $\beta_{A'} = 7.1 \times 10^{-4} \text{ mol}$ dm ⁻³ [3.61.2] and $k_d = *4.0 \times 10^4 \text{ s}^{-1}$ [1.32.9]. | Alga.70E079 |

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

| 2.56.10 | $k_{\rm r} = 2.1 \times 10^{5}$ $k_{\rm r} = 6.5 \times 10^{4}$ c | 1.4×10^{-1} 1.47×10^{-1} | 25 25 30 3–4 | | 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]. 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]. 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]. ${}^{1}O_2^*$ from H ₂ O 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 | Alga.70E079 Alga.70E079 Higg68F29 |
|---|---|--|-----------------------|--------------|---|-----------------------------------|
| 2.56.12 MeOH /t-Bu (1:1) v: 2.56.13 MeOH /r-Bu (1:1) v: 2.56.14 MeOH /t-Bu (1:1) v: 2.56.15 MeOH /t-Bu (1:1) v: For mo. 2.57 4-methylcyclo- hexene | $k_{r} = 1.8 \times 10^{5}$ DH $k_{r} = 2.1 \times 10^{5}$ DH $k_{r} = 6.5 \times 10^{4}$ | 1.47 × 10 ⁻¹ | 30 3-4 | Pa-17 P'a | 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]. 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]. ${}^{1}O_2$ * from $H_2O_2/NaOCl$, A' = 2M2P. Measured $(k_r^{A'}/k_r)$ = 3.9. k_r derived using $k_r^{A'}$ = | Higg68F29 |
| /t-Bu' (1:1) v: 2.56.13 | $k_{\rm r} = 2.1 \times 10^5$ $k_{\rm r} = 6.5 \times 10^4$ $k_{\rm r} = 6.5 \times 10^4$ | | 3–4 | P'a Pa-17 | S = RB, A' = 2M2P. Measured $(k_r^{A'}/k_r)$ = 4.5. k_r derived using $k_r^{A'}$ = *8.1 × 10 ⁵ dm³ mol ⁻¹ s ⁻¹ [A3.3]. ${}^{1}O_2$ * from $H_2O_2/NaOCl$, A' = 2M2P. Measured $(k_r^{A'}/k_r)$ = 3.9. k_r derived using $k_r^{A'}$ = | |
| /t-But (1:1) v: 2.56.14 MeOH /t-But (1:1) v: 2.56.15 MeOH /t-But (1:1) v: For mo. 2.57 4-methylcyclo- hexene | $k_{\rm r} = 6.5 \times 10^4$ | | | | ${}^{1}O_{2}$ * from $H_{2}O_{2}/NaOCl$, A' = 2M2P. Measured $(k_{r}^{A'}/k_{r}) = 3.9$. k_{r} derived using $k_{r}^{A'} =$ | Higg68F29 |
| /t-But (1:1) v: 2.56.15 MeOH /t-But (1:1) v: For mo. 2.57 4-methylcyclo- hexene | OH . | | rt | | $*8.1 \times 10^{5} \text{dm}^{3} \text{mol}^{-3} \text{s}^{-1}$ [A3.3]. | |
| /t-But (1:1) v: For mode 1:57 4-methylcyclo-hexene | | | | Ad-17 A'd | - | Higg68F292 |
| 2.57 4-methylcyclo- MeOH hexene | | | rt | Ad-17 A'd | $^{1}O_{2}*$ from $H_{2}O_{2}/Ca(OCl)_{2}$, 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]. | Higg68F292 |
| hexene | e relative rates see | 2.5, 2.7, 2.43.3-4, 2.75.1, 2.77, 2.84, | | 2.9, 2.59, 2 | 2.64, 2.71, 2.74.6, | |
| | $k_{\rm r}=3.1\times10^3$ | 2.73.1, 2.77, 2.0 4 | 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 × 10 ³ dm ³ mol ⁻¹ s ⁻¹ [2.54.1]. | Kope.65F028 |
| 2.58 1,2-dimethyl- MeOHo cyclohexene | ?) 3.3 × 10 ⁶ | 3.0×10^{-2} | rt | ? | Method not given. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6]$. | Goll62F005 |
| 2.58.1 MeOH | $k_{\rm r}=1.6\times10^7$ | | 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 dm³ 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 | Fig. 1.67 \times 1.67 \times 1.68 \times 1.67 | Monr78A005 |
| For mo | re relative rates see | 2.52. | | | · · · · · · · · · · · · · · · · · · · | |

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

| No. | Substrate (A) | Solvent | /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|-------------------------------------|------------------|--|---------------------------------------|----------|--------------|--|-------------|
| 2.59 | 2,3-dimethyl- cyclohexene | МеОН | $k_{\rm r} = *2.1 \times 10^5$ | | 15 | Ad-17 A'd | S = MB, A' = 1-methyl-cyclohexene. Measured $(k_r/k_r^{A'}) = 1.07 \pm 0.03$. k_r derived using $k_r^{A'} = *2.0 \times 10^5 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [A3.5]. | Kope.65F028 |
| 2.60 | CH | For more MeOH | relative rates see $\approx 1.0 \times 10^5$ | 2.50. ≈ 1.0 | 20 | Od-15 | S = MB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a =$ 13 kJ mol ⁻¹ . | Koch68F288 |
| | ньс снь | | | | | | | |
| 2.61 | terpinolene | МеОН | $\approx 2.0 \times 10^6$ | $\approx 5.0 \times 10^{-2}$ | 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 |
| 2.62 | 3,6-endoperoxy-cyclohexene | МеОН | 6.7×10^2 | 150 | 20 | Od-15 | S = RB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a =$ 26 kJ mol ⁻¹ . | Koch68F288 |
| 2.63 | 1,2-diphenyl- 3,6-dioxacyclohexe | | $k_{\rm r} = 1.3 \times 10^7$ *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]. | Bart70F733 |
| 2.64 | 2-methylnorborn- 2-ene | CH₃CN | $k_{\rm r}=2.8\times10^4$ | | 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]. | Jeff73F664 |
| 2.64.1 | | CH₃CN | $k_{\rm r}=4.0\times10^4$ | | rt | Ad-17 A'd | S = MB, A' = 2-methylidenenorbornane. Measured $(k_r/k_r^{A'})$ = 3.1. k_r derived using $k_r^{A'}$ = 1.3 × 10 ⁴ dm ³ | Jeff.74F647 |
| 2.64.2 | | CH₃CN | $k_{\rm r}=4.9\times10^4$ | | 0 | Ad-17 A'd | mol ⁻¹ s ⁻¹ [2.71]. S = MB, A' = 2-methylidenenorborn-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]. | Jeff78F149 |

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

| No. S | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /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 |
| | OSi (CH ₃) ₃ | | | | | | | |
| 2.66 | 2,7,7-trimethyl- norborn-2-ene | | relative rates see $1.2 	imes 10^4$ | 2.67. 8.2 | ? | ? | Method not given. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6]$. | Goll68F28 |
| | CH ₃ | | | , | | | 1.0 × 10 5 [1.3.0]. | |
| 2.66.1 | | CH₃CN | $k_{\rm r}=1.0\times10^3$ | | rt | Ad-17 A'd | S = MB, A' = 2-methyl- idenenorbornane. Measured (k_r/k_r^A) = 7.7×10^{-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 ₃ CN | $k_{\rm r}=1.2\times10^3$ | | 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 $k_r^{A'} = 4.9 \times 10^4 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [2.64.2]. | Jeff78F14 |
| 2.67 | 7,7-dimethyl-2- (trimethylsiloxy)- norborn-2-ene | CDCl ₃ | $(k_{\rm r}/k_{\rm r}^{\rm A'})=0.12$ | | rt | Ad-17 A'd | S = $meso$ -TPP, A' = 2-(trimethyl-siloxy)norborn-2-ene. | Jeff.78F290 |
| | OSi (CH ₃) ₃ | | | | | | | |
| 2.68 | Δ ² -carene | | relative rates see 5.9×10^5 | $2.65, 2.95, 2.96.$ 1.7×10^{-1} | rt | ? | Method not reported. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [I.3.6]$. | Goll68F289 |
| | CH ₃ | | | | | | | |
| 2.69 | Δ³-carene | MeOH(?) | 2.5×10^5 | 4.0 × 10 ⁻¹ | rt | ? | Method not reported. k derived using $k_d = 1.0 \times 10^5 \text{ s}^{-1} [1.3.6]$. | Goll68F289 |
| | CH ₃ | | | | | | | |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /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 $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6]$. | Goll68F289 |
| 2.71 | 2-methylidene- norbornane | CH ₃ CN | $k_{\rm r}=1.3\times10^4$ | | rt | ? | S = MB, A' = 1-methyl-cyclohexene. Measured $(k_r/k_r^{A'}) = 0.65$. k_r derived using $k_r^{A'} = *2.0 \times 10^5 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [A3.5]. | Jeff73F66 |
| 2.71.1 | | CH₃CN | $k_r = 1.5 \times 10^4$ | | 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 × 10 ³ dm ³ mol ⁻¹ s ⁻¹ [2.94b]. | Jeff78F149 |
| 2.71.2 | | CH ₃ CN | $k_{\rm r}=1.6\times10^4$ | | 0 | Ad-17 A'd | | Jeff78F149 |
| 2.72 | exo-2- methylidene- norbornane-3-d | | relative rates see $k_{\rm r} = 1.5 \times 10^4$ | 2.64.1, 2.72, 2.73, 2 | 2.74.7, 2.75 rt | 5.2. Ad-17 A'd | S = MB, A' = 2-methylidenenorbornane. Measured $(k_r/k_r^{A'})$ = 1.14 ± 0.01. k_r derived using $k_r^{A'}$ = 1.3 × 10 ⁴ dm ³ mol ⁻¹ s ⁻¹ [2.71]. | Jeff.74F647 |
| 2.73 | endo-2- methylidene- norbornane-3-d | CH ₃ CN | $k_{\rm r}=1.3\times10^4$ | | rt | Ad-17 A'd | S = MB, A' = 2-methylidenenorbornane. Measured $(k_r/k_r^{A'})$ = 1.02 ± 0.01 . k_r derived using $k_r^{A'}$ = 1.3×10^4 | Jeff.74F647 |
| 2.74 | α-pinene CH ₃ H ₃ C | MeOH(?) | 1.2×10^4 | 8.2 | rt | ? | dm ³ mol ⁻¹ s ⁻¹ [2.71]. Method not reported. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Goll68F289 |
| 2.74.1 | | MeOH | 2.0 × 10 ⁴ | 5.0 | 20 | Od-15 | S = RB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a =$ 19 kJ mol ⁻¹ . | Koch68F288 |
| 2.74.2 | | МеОН | 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 | | МеОН | 2.0×10^5 | 5.0 × 10 ⁻¹ | 20 | Od-15 | $E_a = 17 \text{ kJ mol}^{-1}$. S = tetrachloro- fluorescein. k derived using $k_d =$ *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. $E_a = 17 \text{ kJ mol}^{-1}$. | Koch68F288 |

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

| No. S | Substrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|--|--|--|---------------------------------------|----------|--------------|---|-------------|
| 2.74.4 | | МеОН | 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]. $E_a = 20 \text{ kJ mol}^{-1}$. | Koch68F28 |
| 2.74.5 | | МеОН | 3.6×10^4 | 2.8 | 20 | Od-15 | | Koch68F28 |
| 2.74.6 | | CH ₃ CN | $k_{\rm r}=5.0\times10^4$ | | rt | ? | $S_a = MB$, $A' = 1$ -methyl-cyclohexene. Measured $(k_r/k_r^{A'}) = 0.25$. k_r derived using $k_r^{A'} = *2.0 \times 10^5 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [A3.5]. | Jeff73F66 |
| 2.75 | β-pinene CH ₂ H ₂ H ₃ H ₄ CH ₂ | МеОН | $\approx 1.0 \times 10^5$ | ≈ 1.0 | 20 | Od-15 | | Koch68F288 |
| 2.75.1 | | CH₃CN | $k_{\rm r}=3.8\times10^4$ | | · rt | Ad-17 A'd | S = MB, A' = 1-methyl-cyclohexene. Measured $(k_r/k_r^{A'}) = 0.19$. k_r derived using $k_r^{A'} = *2.0 \times 10^5 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [A3.5]. | Jeff73F66 |
| 2.75a | 7,7-dimethyl-2-methylidene-norbornane | CH ₃ CN | $k_{\rm r}=3.4\times10^3$ | | 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 $k_r^{A'}$ = 1.3×10^4 dm ³ mol ⁻¹ s ⁻¹ [2.71]. | Jeff.74F647 |
| 2.75a.1 | | CH ₃ CN | $k_{\rm r}=4.1\times10^3$ | | 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 $k_r^A = 1.2 \times 10^3 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [2.66.2]. | Jeff78F149 |
| 2.76 | 1-heptene $CH_3(CH_2)_4CH \approx CH_3(CH_2)_4CH \approx CH_3(CH_2)_5CH \approx CH_3(CH_2)$ | | OH $(1.5 \pm 0.5) \times 10^3$ | | rt | A'd-8 | S = MB, $A' = DPBF$, ruby laser (694 nm). | Bort77F16 |
| 2.77 | 1-methylcyclo- heptene | ? | $k_{\rm r}=1.9\times10^6$ | | rt | ? | Experimental method unclear, A' = 1-methyl-cyclohexene. Measured $(k_r/k_r^{A'}) = 9.4$. k_r derived using $k_r^{A'} = *2.0 \times 10^5 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [A3.5]. | Foot.71F580 |
| 2.78 | trans-4-methyl- 4-octene $CH_3(CH_2)_2CH = C(0$ | MeOH CH ₃)(CH ₂); | 5.0×10^5 ${}_{2}$ CH ₃ | 2.0×10^{-1} | -20 | Od-14 27 | S = RB, A' = α -terpinene. k derived using $k_d = *1.0 \times 10^5$ | Chai.76F909 |
| 2.79 | cis-4-methyl- 4-octene $CH_3(CH_2)_2CH = C(0$ | MeOH CH ₃)(CH ₂); | 3.3×10^5 ${}_{2}\text{CH}_{3}$ | 3.4×10^{-1} | -20 | Od-14 27 | s ⁻¹ [1.3.6]. 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. S | Substrate (A) | Solvent | k /dm³ mol-1 s-1 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|-------------------------------|--|---------------------------------------|----------|--------------|--|-------------|
| 2.80 | 4-methyl-4-octene (46% trans,54% cis) | | 3.7 × 10 ⁵ | 2.7 × 10 ⁻¹ | -20 | Od-14 27 | S = RB, A' = α -terpinene. k derived using $k_d = *1.0 \times 10^5$ | Chai.76F909 |
| 2.81 | 4-methyl-4-octene (25% trans, 75% cis | | 3.4×10^5 | 2.9 × 10 ⁻¹ | -20 | Od14 27 | s ⁻¹ [1.3.6]. 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 | MeOH | 6.25×10^5 | 1.6×10^{-1} | 20 | Pa-15 | S = RB. k derived using $k_d = *1.0 \times 10^5$ | Gol162F005 |
| 2.82.1 | (CH ₃) ₂ C=CHCH ₂ C | MeOH | 6.25×10^{5} | 1.6×10^{-1} | 20 | Pa-15 | s^{-1} [1.3.6]. S = Ery. k derived $u \sin g k_d = *1.0 \times 10^5$ 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 (7:3) v:v | ₂ O 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 ₂ (7:3) v:v | 0 3.5×10 ⁶ (est) | 6.0×10^{-2} | 20 | Pa-15 | S = Eos. k estimated using $k_d = 2.1 \times 10^5 \text{ s}^{-1}$ (calc). | Goll62F005 |
| 2.83 | cyclooctene | EtOH | $(k_{\rm r}/k_{\rm r}^{\rm A'}) = 1.43 \times 10^{-1}$ | | rt | Ad-17 A'd | S = MB, A' = 1,5- cyclooctadiene. | Mats71F58 |
| 2.84 | 1-methylcyclo- octene | ? | $k_{\rm r}=3.0\times10^{\rm 5}$ | | 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 × 10 ⁵ dm ³ mol ⁻¹ | Foot.71F580 |
| 2.85 | 1-nonene CH ₃ (CH ₂) ₆ CH=CH | MeOH I ₂ | $k_{\rm r}=4.6\times10^2$ | | 15 | Ad-17 A'd | s ⁻¹ [A3.5]. S = MB, A' = cyclohexene. Measured $(k_r^{A'}/k_r) = 10$. k_r derived using $k_r^{A'} = 4.6 \times 10^3 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [2.54.1]. | Kope.65F02 |
| 2.86 | cyclopentadiene | МеОН | 2.3×10^{7} | 4.4 × 10 ⁻³ | 20 | Od-15 | S = RB. k derived using $k_d =$ *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. $E_a = 1.3 \text{ kJ mol}^{-1}$. | Koch68F288 |
| 2.86.1 | | МеОН | 2.4×10^7 | 4.1 × 10 ⁻³ | 20 | Od-15 | S = MB. k derived using k_d = *1.0 × 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. 5 | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|-------------------------------------|--|---------------------------------------|----------|--------------|---|-------------|
| 2.86.2 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=3.6\times10^7$ | | 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 [43.2]. | Higg68F29 |
| 2.86.3 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=6.0\times10^7$ | | rt | Ad-17 A'd | O_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 [43.2]. | Higg68F29 |
| 2.86.4 | | MeOH /t-BuOH (1:1) v:v | $k_r = 2.1 \times 10^7$ | | rt | Ad-17 A'd | $^{1}O_{2}^{*}$ from $H_{2}O_{2}/Ca(OCl)_{2}$, $A' = TME$. Measured $(k_{r}/k_{r}^{A'}) = 0.7$. k_{r} derived using $k_{r}^{A'} = *3.0 \times 10^{7} \text{ dm}^{3}$ mol ⁻¹ s ⁻¹ [A3.2]. | Higg68F29 |
| 2.87 | 6,6-dimethyl- fulvene endoperoxi | MeOH ide | $\approx 4.0 \times 10^4$ | ≈ 2.5 | 20 | Od-15 | S = RB. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. E_a = 14 kJ mol ⁻¹ . | Koch68F28 |
| 2.88 | 1,5-hexadiene $CH_2 = CH(CH_2)_2CH $ | (96:4) v:v | H $(2.0 \pm 1.0) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F16 |
| 2.89 | trans,trans-2,4- hexadiene CH ₃ CH=CHCH= | CCl ₄ /MeO (96:4) v:v | H $(2.0 \pm 0.7) \times 10^4$ | | rt | A'd-8 | S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F16 |
| 2.90 | 2,5-dimethyl-2,4- hexadiene (CH ₃) ₂ C=CHCH= | МеОН | $(2.0 \pm 0.5) \times 10^6$ | | rt | A'd-5 | S = MB, A' = DPBF, ruby laser (694 nm). | Merk.72F26 |
| 2.90.1 | (| | $k_{\rm r}=5.6\times10^6$ | | 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 ₂ Cl ₂ | $k_{\rm r}=1.0\times10^6$ | | 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) ₂ CO | $k_{\rm r}=6.4\times10^5$ | | rt | Pa-17 P'a | S = ? A' = 1-methyl- cyclohexene. Measured $(k_r/k_r^{\Lambda'}) = 3.2. k_r$ derived using $k_r^{\Lambda'} =$ *2.0 × 10 ⁵ dm ³ mol ⁻¹ s ⁻¹ [A3.5]. | Hast.73F662 |
| 2.90.4 | | CH ₃ CN | $k_{\rm r}=1.3\times10^6$ | | 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 /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------------|--|---|---------------------------------------|----------|--------------|---|-------------|
| 2.90.5 | MeOH/H (7:3) | $_{2}0 k_{r} = 5.8 \times 10^{6}$ | | 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 ₂ O (3:1) | $k_{\rm r}=2.6\times10^6$ | | rt | Pa–17 P'a | S = ? A' = 1-methyl- cyclohexene. Measured $(k_r/k_r^{A'}) = 13.0. k_r$ derived using $k_r^{A'} = *2.0 \times 10^5 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [A3.5]. | Hast.73F662 |
| 2.91 1,3-cyclohexadiene | МеОН | 2.2 × 10 ⁶ | 4.5 × 10 ⁻² | 20 | Od-15 | S = RB. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. E_a = 5.0 kJ mol ⁻¹ . | Koch68F288 |
| 2.91.1 | МеОН | 4.0 × 10 ⁶ | 2.5 × 10 ⁻² | 20 | Od-15 | S = tetrachloroeosin. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a =$ 5.4 kJ mol ⁻¹ . | Koch68F288 |
| 2.91.2 | МеОН | 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 [1.3.6]. | Koch68F288 |
| 2.91.3 | МеОН | 1.4×10^6 | 7.3×10^{-2} | 20 | Od-15 | $E_{\rm a} = 5.9 \text{ kJ mol}^{-1}.$ S = MB. k derived using $k_{\rm d} =$ *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. $E_{\rm a} = 5.0 \text{ kJ mol}^{-1}.$ | Koch68F288 |
| 2.91.4 | МеОН | 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 [1.3.6]. | Koch68F288 |
| 2.91.5 | MeOH /t-BuOH (1:1) v:v | $k_{\rm r} = 2.3 \times 10^6$ | | rt | Ad-17 A'd | $E_{\rm a} = 5.9 \text{ kJ mol}^{-1}.$ S = RB, A' = TME. Measured $(k_{\rm r}^{A'}/k_{\rm r}) = 13.$ $k_{\rm r}$ derived using $k_{\rm r}^{A'} =$ *3.0 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [43.2]. | Higg68F29 |
| 2.91.6 | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=1.0\times10^7$ | | rt | Ad-17 A'd | The strict $[A3.2]$. $^{1}O_{2}$ * from $H_{2}O_{2}$ /Ca(OCl) ₂ , $A' = TME$. Measured $(k_{r}^{A'}/k_{r}) = 3. k_{r}$ derived using $k_{r}^{A'} = *3.0 \times 10^{7} \text{ dm}^{3}$ $mol^{-1} s^{-1} [A3.2]$. | Higg68F29 |
| 2.92 α-terpinene | МеОН | 1.0×10^{7} | 1.0×10^{-2} | 15 | Od-15 | mol 's ' [A3.2]. S = RB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | Sche.58F004 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|--------------------|--|---------------------------------------|----------|--------------|---|-------------|
| 2.92.1 | | МеОН | 3.2×10^7 | 3.1×10^{-3} | 20 | Od-15 | S = RB. k derived using $k_d =$ | Koch68F28 |
| 2.92.2 | | МеОН | 3.0×10^7 | 3.3 × 10 ⁻³ | 20 | Od~15 | *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. $E_a = 1.7 \text{ kJ mol}^{-1}$. S = tetrachloroeosin. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | Koch68F28 |
| 2.92.3 | | МеОН | 1.7×10^7 | 6.0×10^{-3} | 20 | Od-15 | $E_{\rm a}=1.3~{\rm kJ~mol^{-1}}.$ | Koch68F28 |
| 2.92.4 | | МеОН | 2.5×10^{7} | 4.0×10^{-3} | 20 | Od-15 | using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6].$ | Koch68F28 |
| 2.92.5 | | МеОН | 7.1×10^{7} | 1.4×10^{-3} | 20 | Od-15 | thiophene. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Koch68F28 |
| 2.92.6 | | МеОН | 7.7×10^7 | 1.3 × 10 ⁻³ | 20 | Od-15 | k derived using $k_{\rm d} = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_{\rm a} =$ | Koch68F28 |
| 2.93 | α -phellandrene | МеОН | 1.0 × 10 ⁷ | 1.0×10^{-2} | 20 | Od-15 | 1.7 kJ mol ⁻¹ . S = RB. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. E_a = 4.2 kJ mol ⁻¹ . | Koch68F28 |
| 2.94 | 2,2-dimethyl-cyclohexa-3,5-diene-1-one | МеОН | $\approx 5.3 \times 10^4$ | ≈ 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 . | Koch68F28 |
| 2.94a | 2-methylnorborna- 2,5-diene | CH ₃ CN | $k_{\rm r}=1.2\times10^5$ | | 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 ₃ CN | $k_{\rm r}=3.6\times10^3$ | | 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 | /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|---------------------------------|---|---------------------------------------|----------|-----------------------|--|-------------|
| 2.95 | 2-(trimethyl- siloxy)norborna- 2,5-diene | CDCl ₃ | $(k_{\rm r}/k_{\rm r}^{\rm A'}) = 1.7 \times 10^{-1}$ | | rt | Ad-17 A'd | S = meso-TPP, A' = 7,7-dimethyl-2-(trimethyl-siloxy)norborn-2-ene. | Jeff.78F290 |
| | OSi(CH ₃) ₃ | | | | | | | |
| 2.96 | 7,7-dimethyl-2- (trimethylsiloxy)- norborna-2,5-diene | CDCl ₃ | $(k_{\rm r}/k_{\rm r}^{\rm A'})=4.2$ | | rt | Ad-17 A'd | S = meso-TPP, A' = 7,7-dimethyl-2-(trimethyl-siloxy)norborn-2-ene. | Jeff.78F290 |
| | OSi (CH ₃) ₃ | | | | | | | |
| 2.97 | limonene | MeOH(?) | 5.9 × 10 ⁴ | 1.7 | rt | ? | Method not given. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6].$ | Goll62F005 |
| | H ₃ C CH ₂ | | | | | | | |
| 2.97.1 | | МеОН | 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 . | Koch68F28 |
| 2.98 | nopadiene | МеОН | $\approx 5.0 \times 10^4$ | ≈ 2.0 | 20 | Od-15 | $S = RB \cdot k \text{ derived}$ using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6]$. $E_a = 16 \text{ kJ mol}^{-1}$. | Koch68F28 |
| 2.99 | hexamethyl- bicyclo[2.2.0]- hexa-2,5-diene CH ₃ H ₃ C CH ₃ | CHCl ₃ | $(1.1 \pm 0.2) \times 10^7$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'}$ = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3] and k_{d} = $1.67 \times 10^4 \text{ s}^{-1}$ [1.5]. | Monr78A00 |
| 2.100 | сн ₃ 2,7-dimethyl- 7-hydroperoxy- 2,5-octadiene | МеОН | $k(\text{total}) = 4.2 \times 10^5$ $k(P_1) = 1.9 \times 10^5$ $k(P_2) = 2.3 \times 10^5$ | 2.7 × 10 ⁻¹ | -20 | Od 14 Pa- Ad 27 | $S = RB$, $A' = \alpha$ -terpinene, $P_1 = 2.7$ -dimethyl-2.7-dihydroperoxide-3.5-octadiene, $P_2 = 2.7$ - | Tani.78A35 |
| | (CH ₃) ₂ C(OOH)CH = | | | | | | dimethyl-2,6-dihydro- peroxide-3,7-octadiene. k derived using $k_d = \frac{1}{2} \frac{1}{2$ | |
| 2.101 | 3,7-dimethyl- 1,6-octadiene-2-ol (CH ₃) ₂ C=CH(CH ₂) | MeOH | $(k_r^{A'}/k_r) = 7.3 \times 10^{-2}$ OH)=CH ₃ | | rt | Ad-17 A'd | $1.1 \times 10^{5} \text{ s}^{-1} [1.3.4].$ S = RB, A' = 2,6-di-t-butylphenol. | Mats72F52 |
| 2.101 | | CH ₂ Cl ₂ | $(k_r^{A'}/k_r) = 4.2 \times 10^{-2}$ | | rt | Ad∽17 A′d | ${}^{1}O_{2}^{*}$ from $(PhO)_{3}PO_{3}$ decomposition, $A' = 2,6-di-t$ -butylphenol. | Mats72F52 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|---|---|--|---------------------------------------|----------|-----------------------|---|------------|
| 2.102 | cis-2,6-dimethyl- 2,6-octadiene | МеОН | 1.11 × 10 ⁶ | | -20 | Od-14 27 | S = RB, A' = α -terpinene. k derived using $k_d = 1.1 \times 10^5 \text{ s}^{-1}$ | Tani.78A34 |
| 2.103 | CH ₃ CH = C(CH ₃)(trans-2,6-dimethyl 2,6-octadiene | | $C(CH_3)_2$ 1.85 × 10 ⁶ | | -20 | Od-14 27 | [1.3.4]. S = RB, A' = α -terpinene. k derived using $k_d = 1.1 \times 10^5 \text{ s}^{-1}$ | Tani.78A34 |
| 2.104 | CH ₃ CH=C(CH ₃)(mixture of all monohydroperoxic obtained from pho sensitized oxygena of trans-2,6-dimetl | MeOH les to- tion | $C(CH_3)_2$ 7.4 × 10 ⁵ | | -20 | Od 14 Ad- Pa 27 | [1.3.4]. S = RB, A' = α -terpinene. k derived using k_d = 1.1 × 10 ⁵ s ⁻¹ [1.3.4]. | Tani.78A34 |
| 2.105 | 2,6-octadiene. 2,7-dimethyl- 2,6-octadiene (CH ₃) ₂ C=CH(CH ₂) | MeOH $_{3})_{2}CH = C(C$ | $k(\text{total}) = 1.7 \times 10^{6}$ $k(P_{1}) = 9.0 \times 10^{5}$ $k(P_{2}) = 8.1 \times 10^{5}$ $\text{CH}_{3})_{2}$ | 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 $k_d = 1.1 \times 10^5 \text{ s}^{-1}$ | Tani.78A35 |
| 2.106 | 2,7-dimethyl- 6-hydroperoxy- 2,7-octadiene | МеОН | $k(\text{total}) = 6.0 \times 10^5$ $k(P_1) = 1.9 \times 10^5$ $k(P_2) = 4.1 \times 10^5$ | 1.9 × 10 ⁻¹ | -20 | Od 14 Pa- Ad 27 | [1.3.4]. $S = RB$, $A' = \alpha$ -terpinene. $P_1 = 2.7$ -dimethyl-2.6-dihydroperoxide-3.7-octadiene, $P_2 = 2.7$ -dimethyl-3.6-dihydro- | Tani.78A35 |
| | $CH_2 = C(CH_3)CH(0)$ | OOH)(CH ₂) | | | | | peroxide-1,7-octadiene. k derived using $k_d = 1.1 \times 10^5 \text{ s}^{-1} [1.3.4]$. | |
| 2.107 | trans-2,6,9-tri- methyl-1,6- decadiene | 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 = 6.7×10^4 s ⁻¹ (calc). | Schu78F4 |
| 2.108 | (CH ₃) ₂ CHCH ₂ CH= cis-2,6,9-tri- methyl-1,6- decades | 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 = $6.7 \times 10^4 \text{ s}^{-1}$ (calc). | Schu78F4 |
| 2.109 | (CH ₃) ₂ CHCH ₂ CH= trans-2,6-di- methyl-1,6- undecadiene | 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 = $6.7 \times 10^4 \text{ s}^{-1}$ (calc). | Schu78F4 |
| 2.110 | $CH_3(CH_2)_3CH = C($ cis-2,6-dimethyl- 1,6-undecadiene | (CH ₃)(CH ₂) ₃ EtOH /i-PrOH (1:1) v:v | $3C(CH_3) = CH_2$ 5.2 × 10 ⁵ (est) | 1.3×10^{-1} | 19 | Od-14 27 | S = RB, A' = DMF. k estimated using k_d = 6.7×10^4 s ⁻¹ (calc). | Schu78F4 |
| 2.111 | CH ₃ (CH ₂) ₃ CH = C((-)-caryophyllene | | $_{3}C(CH_{3}) = CH_{2}$ $(k_{r}/k_{r}) = 5.1$ | | 20 | Ad-17 A'd | S = BP, triphenylene, quinoline,Naph,Py, RB,MB; A' = (-)- isocaryophyllene. | Goll70F7 |
| | H ₃ C - CH ₃ CH ₃ | | | | | | | |
| 2.112 | trans-trans-4,8- dimethyl-4,8- dodecadiene CH ₃ (CH ₂),CH=C(| MeOH | 1.11×10^6 $_{2}$ CH=C(CH ₃)(CH ₂) ₂ | .СН ₃ | -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.78A34 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /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 | МеОН | 6.94 × 10 ⁵ | | -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 |
| 2.114 | | to- | 3.82×10^{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 |
| 2.115 | | МеОН | 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 ₃ CH=C(CH ₃)C | МеОН СН=СНСН | 1.4×10^6 = C(CH ₃) ₂ | 7.0×10^{-2} | 20 | Od-15 | S = RB. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6].$ | Koch68F288 |
| 2.117 | cyclooctatetraene dibromide | МеОН | $\approx 3.3 \times 10^{5}$ | $\approx 3.0 \times 10^{-1}$ | 20 | Od-15 | $E_{\rm a} = 8.4 \text{ kJ mol}^{-1}$. S = RB. k derived using $k_{\rm d} = *1.0 \times 10^5$. $s^{-1} [1.3.6]$. $E_{\rm a} = 11 \text{ kJ mol}^{-1}$. | Koch68F288 |
| 2.118 | sarcina phytoene (3 conj. bonds) | C ₆ H ₆ /Me((3:2) v:v | OH<1.9×10 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). | Math74F04 |
| 2.119 | all trans-retinol | C ₆ H ₆ /MeC (4:1) v:v | OH < 7.3 × 10° | | rt | Pa-20 | S = MB, A' = 2M2P. Measured (k/k_A) \leq 9. k derived using $k_{A'} = *8.1 \times 10^5 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [43.3]. | Foot70F18 |
| 2.120 | sarcina phytofluene | C ₆ H ₆ /MeO (3:2) v:v | OH < 1.0 × 10 ⁸ (est) | > 1.0 × 10 ⁻³ | rt | A'd-22 | S = MB, A' = Rub. k estimated using k_d = $1.0 \times 10^5 \text{ s}^{-1}$ (calc). | Math74F04 |
| 2.121 | C-30 carotene analog | C ₆ H ₆ /MeO (4:1) v:v | DH 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]. | Foot70F188 |
| 2.122 | P-422 (8 conj. bonds) | C ₆ H ₆ /MeO (3:2) v:v | $\begin{array}{c} \text{OH} 1.2 \times 10^{10} \\ \text{(est)} \end{array}$ | 8.3 × 10 ⁻⁶ | rt | A'd-22 | S = MB, A' = Rub. k estimated using k_d = $1.0 \times 10^5 \text{ s}^{-1}$ (calc). | Math74F04 |

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

| No. | Substrate (A) | Solvent k /dm³ mo | | t /°C | Method | Comments | Ref. |
|---------|--|---|---|----------|--------|---|-------------|
| 2.123 | C-35 carotene analog | C ₆ H ₆ /MeOH 1.5 × (4:1) v:v | < 10° | 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]. | Foot70F188 |
| 2.124 | P-438 (probably sarcina-xanthin- 9 conj. bonds) | $C_6H_6/MeOH$ 3.1 \times (3:2) v:v (est) | $< 10^{10}$ 3.2 \times 10 ⁻⁶ | rt | A'd-22 | S = MB, A' = Rub. k estimated using k_d = 1.0×10^5 s ⁻¹ (calc). | Math74F04 |
| 2.125 | β-apo-8'- carotenal | C_6H_6 (1.4 ± 0. | $2) \times 10^{10}$ | rt | Ad-12 | S = An, ruby laser (347 nm). | Wilk.78F276 |
| | | ~~~ сно | | | | | |
| 2.126 | β-apo-8'- carotenol | $C_6H_6/MeOH \approx 1.5$ (4:1) v:v | | rt | P'a-20 | S = MB, A' = 2M2P. Measured $(k/k_A) \approx 1900$. k derived using $k_{A'} = *8.1 \times 10^5$ | Foot70F188 |
| | | | CH2OH | | | $dm^3 mol^{-1} s^{-1} [A3.3].$ | |
| 2.126. | 1 | $C_6H_6/MeOH$ 1.2 × (4:1) v:v | < 10 ¹⁰ | 25 | P'a-20 | S= MB, A' = 2M2P. Measured $(k/k_{A'}) \approx 1.5 \times 10^4$. k derived using $k_{A'} = *8.1 \times 10^5$ | Foot70F73 |
| 2.127 | ethyl-β-apo-8'- carotenoate | C_6H_6 (1.2 ± 0. | $2) \times 10^{10}$ | . rt | Ad-12 | $dm^3 mol^{-1} s^{-1} [A3.3].$ S = An, ruby laser (347 nm). | Wilk.78F276 |
| | | ° - 0CH2CH | 3 | | | | |
| 2.128 | lutein | $C_6H_6/MeOH$ 2.1 × (3:2) v:v (est) | $< 10^{10}$ 4.8×10^{-6} | rt | A'd-22 | S = MB, A' = Rub. k estimated using k_d = $1.0 \times 10^5 \text{ s}^{-1}$ (calc). | Math74F04 |
| | но | Lagraph | | | | | |
| 2.129 | isozeaxanthin | $C_6H_6/MeOH$ 2.9 \times (3:2) v:v (est) | 3.4×10^{-6} | rt | A'd-22 | S = MB, A' = Rub. k estimated using k_d = $1.0 \times 10^5 \text{ s}^{-1}$ (calc). | Math74F04 |
| | но | | OH | | | 1.0 × 10 s (carc). | |
| 2.130 | β-carotene Car | MeOH 1.6 × 10 ¹ | $(6.1 \pm 0.6) \times 10^{-6}$ | 6 rt | A'd-16 | S = RB, A' = DPF. k derived using $k_d = *1.0 \times 10^5$ | Youn71F398 |
| | | | | | | s ⁻¹ [1.3.6]. | |
| 2.130.1 | 1 | CCl_4 (7.0 ± 2. | 1) × 10° | rt | Ld-13 | $S = ?$ k derived using $k_d = 3.5 \times 10^1$ 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 /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|---------------------------------|--|---------------------------------------|----------|--------|--|-------------|
| 2.130.2 | CH ₂ Cl 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 $k_d = 7.3 \times 10^3 s^{-1}$. | Carl73P066 |
| 2.130.3 | CH ₂ Cl ₂ | 1.3 × 10 ¹⁰ (est) | | 25 | A'd-23 | S = A' = Rub. k estimated using $k_{A'} = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 8.0 \times 10^3 \text{ s}^{-1}$. | Carl74F341 |
| 2.130.4 | CH ₂ Cl ₂ | 1.7×10^{10} | | 30 | Od-23 | S = MB, A' = TME. k derived using $k_{A'}$ = *3.0 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [A3.2] and k_{d} = *1.2 × 10 ⁴ s ⁻¹ [1.4.2]. | Taim.76F90 |
| 2.130.5 | CH ₂ Cl ₂ | 4.4 × 10° | | 30 | Od-23 | S = MB, A' = 1,3-cyclo- hexadiene. k derived using $k_{A'} = *3.5 \times 10^6 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [A3.8] and $k_d = *1.2 \times 10^4$ s ⁻¹ [1.4.2]. | Taim.76F92 |
| 2.130.6 | CH ₂ Cl ₂ | 1.9×10^{10} | | 30 | Od-23 | S = MB, A' = Rub. k derived using $k_{A'}$ = *4.2 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [A3.14] and k_{d} = *1.2 × 10 ⁴ s ⁻¹ [1.4.2]. | Taim.76F92 |
| 2.130.7 | CS ₂ | 3.3×10^{10} | 1.5×10^{-7} | rt | P'a-20 | S = TPP, A' = 2M2P. k derived using $k_d = 5.0 \times 10^3 \text{ s}^{-1}$ [1.9]. | Foot72F02 |
| 2.130.8 | CFCl₂− CF₂Cl | 1.4 × 10° | | rt | Ad-36 | 1 O ₂ * from Nd/YAG laser (1065 nm). Measured ($k/k_{\rm O2}$) = (1.1 \pm 0.2) \times 10 ⁶ . k derived using $k_{\rm O2}$ = 1.3 \times 10 ³ dm ³ mol ⁻¹ s ⁻¹ (gas phase value). | Math.72M07 |
| 2.130.9 | n-BuOH | 9.5 × 10° | $(5.5 \pm 0.6) \times 10^{-6}$ | rt | A'd-16 | S = RB, A' = DPF. k derived using $k_d = 5.2 \times 10^4 \text{ s}^{-1}$ [1.24]. | Youn71F39 |
| 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 $k_d = 3.0 \times 10^4 \text{ s}^{-1}$ [1.25]. | Youn71F39 |
| 2.130.11 | C ₅ H ₅ N | 6.5 × 10° | | rt | A'd-23 | S = A' = Rub. k derived using $k_{A'}$ = $4 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{d} = *6.0 \times 10^4 \text{ s}^{-1}$ [1.29.1]. | Fahr74R11 |
| 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.73F43 |
| 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.73F43 |
| 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 |

CHEMICAL KINETICS OF SINGLET OXYGEN IN SOLUTION

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------------------|---|---------------------------------------|----------|--------|--|-------------|
| 2.130.16 | C_6H_5Br 3.4 × 10° (est) | | 0 | A'd-33 | $^{1}O_{2}$ * 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 = 1×10^5 s ⁻¹ (calc) and k_A = 1.7×10^8 dm ³ mol ⁻¹ s ⁻¹ . | Zwei.75P063 |
| 2.130.18 | CCl_4 6.2 × 10 ⁹ /CHCl ₃ (est) (9:1) v:v | | rt | A'd-23 | S = A' = Rub. Measured $k/(k_A[A'] + k_d) =$ $3.5 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ at}$ $[A'] = 5 \times 10^{-6} \text{ mol dm}^{-3}$. $k \text{ estimated using } k_{A'} =$ $7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ and}$ $k_d = 1.43 \times 10^3 \text{ s}^{-1} [1.8]$. | Hrdl74F64 |
| 2.130.18a | EtOH/H ₂ O(2.2 \pm 0.5) \times 10 ⁹ (95:5) v:v | | rt | Ld-13 | ¹ O ₂ * from pyrogallol autooxidation by O ₂ /KOH. k measured by monitoring the quenching of chemiluminescence by A. | Slaw78F605 |
| 2.130.19 | $C_6H_6/MeOH$ 1.2 × 10 ¹⁰ (4:1) v:v | | 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 [43.3]. | Foot70F73 |
| 2.130.20 | $C_6H_6/MeOH$ 9.7 × 10° (4:1) v:v | $(3.9 \pm 0.4) \times 10^{-6}$ | rt | A'd~16 | S = RB, A' = DPF. k derived using $k_d = 3.8 \times 10^4 \text{s}^{-1}$ [1.49]. | Youn71F39 |
| 2.130.21 | $C_6H_6/MeOH$ 2.3 × 10 ¹⁰ (3:2) v:v (est) | 4.3 × 10 ⁻⁶ | rt | A'd-22 | S = MB, A' = Rub. k estimated using k_d = $1.0 \times 10^5 \text{ s}^{-1}$ (calc). | Math74F04 |
| 2.130.22 | C_6H_6/EtOH 1.3 × 10 ¹⁰ (8:1) v:v (est) | | 22 | P'a-13 | S = RB, A' = TMHP, P' = nitroxy radicals. k estimated using k_d = 3×10^4 s ⁻¹ (calc). | Ivan75F44 |
| 2.130.23 | C_6H_6/EtOH 1.65 × 10 ¹⁰ (2:1) v:v (est) | | rt · | A'd-19 | S = RB, A' = chlorophyll-a. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc). | Koka.78F404 |
| 2.131 canthaxanthin | For more relative rates see C_6H_6 (1.45 \pm 0.2) \times 10 10 | 2.55, 4.7.6. | rt | Ad-12 | S = An, ruby laser (347 nm). | Wilk.78F276 |
| 2.132 lycopene | $C_6H_6/MeOH \approx 1.2 \times 10^{10}$ (4:1) v:v | | rt | 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.70F188 |

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

| lo. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | <i>t</i> /°C | Method | Comments | Ref. |
|-------|---|--|---|---------------------------------------|-------------------------|--------------|--|--------------------|
| | | | | rate constant unless | k _r (chemica | | | |
| | | or k _q (quen | ching rate constant) | s specified; $k_{\rm d}$ is the | rate consta | nt for solve | ent deactivation_ | |
| .1 | benzene C ₆ H ₆ | CCl ₄ | $(2.2 \pm 1.5) \times 10^3$ | | rt | A'd-8 | S = MB, $A' = DPBF$, dye laser (610 nm). | Youn.76F9 |
| .1.1 | | CCl ₄ /MeO (96:4) v:v | $0H(5.0 \pm 3.0) \times 10^2$ | | rt | A'd-8 | S = MB, $A' = DPBF$, ruby laser (694 nm). | Bort77F1 |
| .2 | bromobenzene C ₆ H₅Br | CCl ₄ | $(1.9 \pm 1.3) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, dye laser (610 nm). | Youn.76F9 |
| .3 | ethylbenzene C ₆ H ₅ C ₂ H ₅ | CCl ₄ /MeC (96:4) v:v | $0H(5.0 \pm 3.0) \times 10^2$ | | rt | A'd-8 | S = MB, $A' = DPBF$, ruby laser (694 nm). | Bort77F1 |
| .4 ` | methoxybenzene C ₆ H ₅ OCH ₃ | МеОН | $k_{\rm r} \leqslant 5 \times 10^6$ (est) | | 20 | Ad-17 A'd | S = RB, and MB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect. | Sait72A02 |
| 3.5 | methyl benzoate C ₆ H ₅ COOCH ₃ | CCI ₄ | $(2.9 \pm 1.8) \times 10^3$ | | . rt | A'd-8 | S = MB, A' = DPBF, dye laser (610 nm). | Youn.76F9 |
| .6 | styrene $C_6H_5CH=CH_2$ | CCl₄/MeC (96:4) v:v | $0H(5.0 \pm 2.0) \times 10^3$ | | rt | A'd-8 | S = MB, $A' = DPBF$, ruby laser (694 nm). | Bort77F1 |
| 3.7 | $cis-\beta$ -methyl- styrene $C_6H_5CH=CHCH_3$ | (96:4) v:v | $0H(5.0 \pm 1.5) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F1 |
| .8 | trans- β -methyl- styrene $C_6H_5CH=CHCH_3$ | CCl ₄ /MeO (96:4) v:v | $0H(2.0 \pm 1.0) \times 10^3$ | | rt | A'd-8 | S = MB, $A' = DPBF$, ruby laser (694 nm). | Bort.77F16 |
| .9 | 3-methyl-1- phenyl-2-butene $C_6H_5CH_2CH=C(C)$ | MeOH(?) | 7.7×10^{5} | 1.3×10^{-1} | ŗt | ? | Method not given. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6].$ | Goll62F00 |
| .9.1 | | MeOH | 6.7×10^{5} | 1.5 × 10 ⁻¹ | 20 | Od-15 | $K_d = 1.0 \times 10^{5} \text{ s}^{-1} [1.3.6].$ S = RB. k derived using $k_d = *1.0 \times 10^{5}$ $s^{-1} [1.3.6]. E_a = 9.6$ kJ mol ⁻¹ . | Koch68F2 |
| | | | COMI | POUNDS 3,10 - 3,19 | 9 : | | | ř |
| | | | | e C(CH3) = C(CH3)2 | | | | |
| 3.10 | trimethylstyrene (TMS) | MeOH /C ₅ H ₅ N (98:2) v:v | $k_{\rm r}=5.0\times10^6$ | | 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 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [3.18]. | Foot.71F57 |
| .10. | 1 | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=4.8\times10^6$ | | rt | Pa-17 P'a | $^{1}O_{2}*$ from $H_{2}O_{2}/NaOCl$, A' = p-methoxytrimethyl- styrene. Measured. $(k_{r}/k_{r}^{A'}) = 0.57$. k_{r} derived using $k_{r}^{A'} =$ $8.4 \times 10^{6} \text{ dm}^{3} \text{ mol}^{-1}$ | Foot.71F5 |
| . 10. | 2 | MeOH /t-BuOH (1:1) v:v | $k_{\rm r} = 5.2 \times 10^6$ | | rt | Pa-17 P'a | s ⁻¹ [3.18.1]. ¹ O ₂ * from H ₂ O ₂ /NaOCl, A' = p-methyltrimethylstyn Measured $(k_r^{A'}/k_r)$ = 1.20. k_r derived using $k_r^{A'}$ = 6.3 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [3.13.1]. | Foot.71F5 rene. |
| | | For more i | 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 /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|--|---|--|--------------|--------------|---|------------|
| 3.11 | m-chlorotri- methylstyrene [$R_3 = -C1$] | MeOH /C ₅ H ₅ N (98:2) v:v | $k_{\rm r}=2.8\times10^6$ | | rt | Pa-17 P'a | S = RB, A' = p-methyl-trimethylstyrene. Measured $(k_r/k_r^{A'})$ = 0.384. k_r derived using $k_r^{A'}$ = 7.2 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [3.13]. | Foot.71F57 |
| 3.11.1 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=2.7\times10^6$ | | rt | Pa-17 P'a | $^{1}O_{2}^{*}$ from $H_{2}O_{2}/NaOCl$, A' = p-methyltri- methylstyrene. Measured $(k_{r}/k_{r}^{A'}) = 0.436$. k_{r} derived using $k_{r}^{A'} =$ 6.3×10^{6} dm ³ mol ⁻¹ s ⁻¹ [3.13.1]. | Foot.71F57 |
| 3.12 | p-chlorotri- methylstyrene [$R_4 = -C1$] | МеОН | $k_r = 3.3 \times 10^6$ | | rt | Pa-17 P'a | S = RB, A' = 2-methyl- 2-butene. Measured $(k_r/k_r^{A'}) = 2.23$. k_r derived using $k_r^{A'} = *1.5 \times 10^6 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [A3.1]. | Foot.71F57 |
| 3.13 | p-methyltri- methylstyrene [$R_4 = -Me$] | For more r MeOH /C ₅ H ₅ N (98:2) v:v | elative rates see $k_{\rm r} = 7.2 \times 10^6$ | 3.13, 3.13.1, 3.14, 3 | .14.1. rt | Pa-17 P'a | S = RB, A' = p -cloro- trimethylstyrene. 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.71F57 |
| 3.13.1 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=6.3\times10^6$ | | rt | Pa-17 P'a | $^{1}O_{2}*$ from $H_{2}O_{2}/NaOCl$, A' = p-chlorotrimethyl- styrene. Measured $(k_{r}^{A'}/k_{r}) = 0.526$. k_{r} derived using $k_{r}^{A'} = 3.3 \times 10^{6} \text{ dm}^{3} \text{ mol}^{-1}$ $s^{-1} [3.12]$. | Foot.71F57 |
| | | For more r | elative rates see | 3.10.2, 3.11, 3.11.1, 3.17.1, 3.18, 3.18.1. | | 6, 3.16.1, 3 | .17, | |
| 3.14 | m-methyltri- methylstyrene [$R_3 = -Me$] | MeOH /C ₅ H ₅ N (98:2) v:v | $k_{\rm r}=5.1\times10^6$ | | rt | Pa–17 P'a | S = RB, A' = p-chloro- trimethylstyrene. Measured $(k_r/k_r^{A'})$ = 1.54. k_r derived using $k_r^{A'}$ = 3.3 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [3.12]. | Foot.71F57 |
| 3.14.1 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=4.7\times10^{\rm o}$ | | rt | Pa–17 P'a | $^{1}O_{2}*$ from $H_{2}O_{2}/NaOCl$, A' = p-chlorotrimethyl- styrene. Measured $(k_{r}/k_{r}^{A'}) = 1.43. k_{r}$ derived using $k_{r}^{A'} = 3.3 \times 10^{6} \text{ dm}^{3} \text{ mol}^{-1}$ $s^{-1} [3.12]$. | Foot.71F57 |
| 3.15 | m-cyanotri- methylstyrene [$R_3 = -CN$] | MeOH /C ₅ H ₅ N (98:2) v:v | $k_r = 1.4 \times 10^6$ | | rt | Pa-17 P'a | S = RB, A' = p-methyl- trimethylstyrene. Measured $(k_r/k_r^{A'})$ = 0.197. k_r derived using $k_r^{A'}$ = 7.2 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [3.13]. | Foot.71F57 |
| 3.15.1 |) | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=1.6\times10^6$ | | rt | Pa-17 P'a | $^{1}O_{2}*$ from $H_{2}O_{2}/NaOCl$, A' = p-methyltrimethyl- styrene. Measured $(k_{r}/k_{r}^{A'}) = 0.252$. k_{r} derived using $k_{r}^{A'} =$ $6.3 \times 10^{6} \text{ dm}^{3} \text{ mol}^{-1}$ s^{-1} [3.13.1]. | Foot.71F57 |

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

| No. S | Substrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|--|--|---------------------------------------|----------|--------------|--|------------|
| 3.16 | p -cyanotri- methylstyrene $[R_4 = -CN]$ | MeOH /t-BuOH (98:2) v:v | $k_{\rm r}=1.2\times10^6$ | | rt | Pa-17 P'a | S = RB, A' = p-methyl- trimethylstyrene. Measured $(k_r/k_r^{A'})$ = 0.172. k_r derived using $k_r^{A'}$ = 7.2 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [3.13]. | Foot.71F57 |
| 3.16.1 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=9.7\times10^5$ | | rt | Pa~17 P'a | In the form $H_2O_2/NaOCl$ A' = p-methyltrimethylstyrene. Measured $(k_r/k_r^{A'}) = 0.154$. k_r derived using $k_r^{A'} = 6.3 \times 10^6$ dm ³ mol ⁻¹ s ⁻¹ [3.13.1]. | Foot.71F57 |
| 3.17 | m-methoxytri- methylstyrene [$R_3 = -OMe$] | MeOH /C ₅ H ₅ N (98:2) v:v | $k_{\rm r}=4.8\times10^6$ | | rt | Pa-17 P'a | S = RB, A' = p -methyl- trimethylstyrene. Measured $(k_r/k_r^{A'})$ = 0.667. k_r derived using $k_r^{A'}$ = 7.2 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [3.13]. | Foot.71F57 |
| 3.17.1 | | MeOH /t-BuOH (1:1) v:v | $k_r = 5.2 \times 10^6$ | | rt | Pa-17 P'a | $^{1}O_{2}*$ from $H_{2}O_{2}/NaOCl$, A' = p-methyltrimethyl- styrene. 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.71F57 |
| 3.18 | p-methoxytri- methylstyrene [R ₄ = -OMe] | MeOH /C ₅ H ₅ N (98:2) v:v | $k_{\rm r}=9.9\times10^6$ | | rt | Pa-17 P'a | S = RB, A' = p -methyl-trimethylstryene. Measured $(k_r/k_r^{A'})$ = 1.38. k_r derived using $k_r^{A'}$ = 7.2 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [3.13]. | Foot.71F57 |
| 3.18.1 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=8.4\times10^6$ | | rt | Pa-17 P'a | $^{1}O_{2}*$ from $H_{2}O_{2}/NaOCl$, $A' = p$ -methyltrimethylstyrene. Measured $(k_{r}/k_{r}^{A'}) = 1.33. k_{r}$ derived using $k_{r}^{A'} = 6.3 \times 10^{6} \text{ dm}^{3} \text{ mol}^{-1}$ s ⁻¹ [3.13.1]. | Foot.71F57 |
| | | | elative rates see | 3.10, 3.10.1, 3.19, 3. | 19.1. | | | |
| 3.19 | p-(N , N -dimethyl- amino)trimethyl- styrene [$R_4 = -N(CH_3)_2$] | MeOH /C₅H₅N (98:2) v:v | $k_{\rm r}=2.0\times10^7$ | | rt | Pa-17 P'a | S = RB, A' = p-methoxy- trimethylstryene. Measured $(k_r/k_r^{A'})$ = 2.0. k_r derived using $k_r^{A'}$ = 9.9 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [3.18]. | Foot.71F57 |
| 3.19.1 | | MeOH /t-BuOH (1:1) v:v | $k_{\rm r}=2.4\times10^7$ | | rt | Pa-17 P'a | $^{1}O_{2}*$ from $H_{2}O_{2}/$ NaOCl, A' = p-methoxytrimethyl- styrene. Measured $(k_{r}/k_{r}^{A'}) = 2.9. k_{r}$ derived using $k_{r}^{A'} =$ $8.4 \times 10^{6} \text{ dm}^{3} \text{ mol}^{-1}$ $s^{-1} [3.18.1].$ | Foot.71F57 |
| 3.20 | 1-cyclopropyl-2- methyl-1-phenyl- propene | (Me) ₂ CO | $k_{\rm r}=1.2\times10^6$ | | rt | Ad-17 A'd | S = Eos, A' = (dicyclo- propylmethylidene cyclobutane. Measured $(k_r/k_r^A) = 0.79$. k_r derived using $k_r^{A'} =$ | Rous78F43 |
| | (CH ₃) ₂ C = C | | | | | | 1.5 × 10 ⁶ dm ³ mol ⁻¹ s ⁻¹ [2.19.4]. | |

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

| No. | Substrate (A) | Solvent | /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | /°C | Method | Comments | Ref. |
|------|--|-------------------------------------|--|---------------------------------------|-----|--------------|--|------------|
| 3.21 | cis-stilbene | • | $OH(3.0 \pm 1.5) \times 10^3$ | | rt | A'd-8 | A = MB, A' = DPBF, | Bort77F16 |
| 3.22 | $C_6H_5CH = CHC_6H_5$ $cis-\alpha$ -methyl- stilbene | CCl ₄ /MeC (96:4) v:v | $0\text{H}(6.0 \pm 2.5) \times 10^3$ | | rt | A'd-8 | ruby laser (694 nm). S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F16 |
| 3.23 | $C_6H_5C(CH_3) = CHC$ trans- α -methyl- stilbene | CCl ₄ /MeC (96:4) v:v | $0H(3.0 \pm 1.5) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F16 |
| 3.24 | $C_6H_5C(CH_3) = CHC$ 1,2-dimethoxy- stilbene $C_6H_5C(OCH_3) = C(OCH_3)$ | (Me) ₂ CO | $k_{\rm r} = 9.7 \times 10^6$ *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 ×10 ⁵ (*1.8 × 10 ⁵) dm ³ mol ⁻¹ s ⁻¹ [2.55.1]. | Bart70F733 |
| 3.25 | 1,2-dimethoxy- benzene 1,2-C ₆ H ₄ (OCH ₃) ₂ | MeOH | $k_{\rm r} \leqslant 5 \times 10^6$ (est) | | 20 | Ad-17 A'd | S = RB and MB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect. | Sait72A020 |
| 3.26 | 1,3-dimethoxy- benzene 1,3-C ₆ H ₄ (OCH ₃) ₂ | МеОН | $k_r \leqslant 5 \times 10^6$ (est) | | 20 | Ad-17 A'd | S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect. | Sait72A020 |
| 3.27 | 1,4-dimethoxy- benzene 1,4-C ₆ H ₄ (OCH ₃) ₂ | МеОН | $k_{\rm r} \leqslant 5 \times 10^6$ (est) | | 20 | Ad-17 A'd | S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect. | Sait72A020 |
| 3.28 | anethole CH = CHCH ₃ OCH ₃ | МеОН | $\approx 1.0 \times 10^7$ | $\approx 1.0 \times 10^{-2}$ | 20 | Od-15 | S = RB. k derived using $k_d = *1.0 \times 10^5$ $s^{-1}[1.3.6]$. $E_a = 17$ kJ mol ⁻¹ . | Koch68F288 |
| 3.29 | 1,2,3-trimethoxy- benzene 1,2,3-C ₆ H ₃ (OCH ₃) ₃ | МеОН | $k_{\rm r} \leqslant 5 \times 10^6$ (est) | | 20 | Ad-17 A'd | S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect. | Sait72A020 |
| 3.30 | 1,2,4-trimethoxy- benzene 1,2,4-C ₆ H ₃ (OCH ₃) ₃ | МеОН | 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])*. | Thom.78A17 |
| | | For more r | elative rates see | 3.34. | | | (j/ · | |
| 3.31 | 1,3,5-trimethoxy- benzene 1,3,5-C ₆ H ₃ (OCH ₃) ₃ | МеОН | $k_{\rm r} \leqslant 5 \times 10^6$ (est) | | 20 | Ad-17 A'd | S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect. | Sait72A020 |
| 3.32 | 1,2,3,4-tetra- methoxybenzene 1,2,3,4-C ₆ H ₂ (OCH ₃) | MeOH | $k_{\rm r} \leqslant 5 \times 10^6$ (est) | | 20 | Ad-17 A'd | S = MB and RB, A' = 1,2,4,5-tetramethoxy-benzene. No measurable effect. | Sait72A020 |
| 3.33 | 1,2,3,5-tetra- methoxybenzene 1,2,3,5-C ₆ H ₂ (OCH ₃) | MeOH | $k_{\rm r}=3.1\times10^7$ | | 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 $k_r^{A'} = 2.1 \times 10^8 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [3.34]. k_r is a mean for runs using both S. | Sait72A020 |

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

| No. S | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|--|---|---------------------------------------|--------------|--------------|---|-------------|
| 3.34 | 1,2,4,5-tetra- methoxybenzene 1,2,4,5-C ₆ H ₂ (OCH ₃) | MeOH | $k_{\rm r}=2.1\times10^8$ | | 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. | Sait72A020 |
| | | For more r | elative rates see | 3.25-7, 3.29, 3.31-3 | 3, 3.37, 3.3 | 9. | 5 | |
| 3.35 | 1,3-dimethoxy- 4,6-di-t-butyl benzene OCH ₃ (CH ₃) ₃ C OCH ₃ | MeOH(?) | $k_{\rm r} = 7.0 \times 10^4$ | | 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]. | Sait70F454 |
| 3.35.1 | Ciongia | MeOH(?) | $k_{\rm r}=9.0\times10^4$ | | rt | Pa-17 P'a | $^{1}O_{2}$ * from H ₂ O ₂ /NaOCl, A' = TME. Measured $(k_{r}/k_{r}^{A'}) = 3.0 \times 10^{-3}$. k_{r} derived using $k_{r}^{A'} = *3.0 \times 10^{7}$ dm ³ mol ⁻¹ s^{-1} [A3.2]. | Sait70F454 |
| 3.36 | 2,6-di- t -butyl- 4-methylanisole $(CH_3)_3$ C $(CH_3)_3$ C $(CH_3)_3$ | МеОН | 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.78A17 |
| 3.37 | pentamethoxy- benzene 1,2,3,4,5-C ₆ H(OCH | MeOH ₃) ₅ | $k_{\rm r}=4.1\times10^7$ | | 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 $k_r^{A'} = 2.1 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.34]. k is a mean | Sait72A020 |
| 3.38 | tetraphenyleyelo- pentadienone | CCl₂F− CCIF₂ | 8.9×10^{6} . $k_{\rm r} = 3.3 \times 10^{6}$ $k_{\rm q} = 5.6 \times 10^{6}$ | 5.3 × 10 ⁻⁵ | 25 | Ad-34 | for runs using both S. ${}^{1}O_{2}^{*}$ from Nd-YAG laser (1065 nm), A' = DPBF. Measured $(k_{q}/k_{r}) = 1.7$. k , k_{r} , and k_{q} derived using $k_{d} = 4.7 \times 10^{2} \text{ s}^{-1} ([1(a).2];$ | Evan.76F417 |
| 3.38.1 | | CCl ₂ F- CClF ₂ | $k_r = 2.8 \times 10^6$ (est) | | rt | Ad-36 | [I(a).2.1]) ^a . ¹ O ₂ * directly from CW Nd-YAG laser (1065 nm). Measured $(k_r/k_{O2} O_2) = 700 \text{ dm}^3 \text{ mol}^{-1}$. k_r estimated using $k_{O2} O_2 = 4 \times 10^3 \text{ s}^{-1}$ (based on gas phase value of $k_{O2} = 1.3 \times 10^3 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$). | 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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|---|--|---------------------------------------|----------|--------------|---|-------------|
| 3.39 | hexamethoxy- benzene 1,2,3,4,5,6-C ₆ (OCF | MeOH | $k_{\rm r}=6.5\times10^6$ | | 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. | Sait72A020 |
| 3.39a | 1,4-dimethoxy- benzonorbornene | C ₆ H ₆ /MeOH (3:1) v:v | 6 × 10 ⁶ | | 25 | A'd-20 | S = RB, A' = cyclohexene. k derived using $\beta_{A'} = 3.1 \text{ mol}^{-1} \text{ dm}^{-3}$ [2.54.3] and $k_d = 6.25 \times 10^4 \text{ s}^{-1}$. | Kret.78F586 |
| 3.40 | indene | МеОН | 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 | | МеОН | 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 ₆ H ₁₂ | $k_{\rm r}=1.2\times10^4$ | | 25 | Ad-17 A'd | S = A' = An. Measured $(k_r/k_r^{A'}) = 7.5 \times 10^{-2}$. k_r derived using $k_r^{A'} = 1.6 \times 10^5 \text{ dm}^3 \text{ mol}^{-1}$ $\text{s}^{-1} [3.44.9]$. | Stev74F312 |
| 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.78F40 |
| 3.43 | 9,9'-bifluorenyl-idene | CH ₂ Cl ₂ | $k_{\rm r}=1.0\times10^6$ | | rt | Ad-17 A'd | S = MB, A' = TME. Measured $(k_r/k_r^{A'})$ = 3.4×10^{-2} . k_r derived using $k_r^{A'}$ = *3.0 × 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 | $^{1}O_{2}$ * from $H_{2}O_{2}/NaOCl$, A' = TME. Measured $(k_{r}/k_{r}^{A'}) = 3.4 \times 10^{-2}$. k_{r} derived using $k_{r}^{A'} =$ *3.0 × 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 /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|---|--|---------------------------------------|----------|--------|--|------------|
| | | COMPOUN | IDS 3.44 – 3.59 : | | | - | |
| | | 7 | 9 1 2 2 3 3 | | | | |
| anthracene (An) | CHCl ₃ | 7.4×10^5 | 1.36×10^{-2} | rt | Od-15 | S = self. k derived using $k_d = *1.0 \times 10^4$ s ⁻¹ [1.5.3]. | Bowe53F00 |
| 3.44.1 | CHCl ₃ | 2.8×10^5 | 3.6×10^{-2} | rt | Pa-15 | S = self. k derived using $k_d = *1.0 \times 10^4$ s^{-1} [1.5.3]. | Bowe55F00 |
| 4.44.2 | CHCl ₃ | $(5.4 \pm 0.6) \times 10^{5}$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ $[3.63.3] \text{ and } k_{d} = 1.67 \times 10^4 \text{ s}^{-1} [1.5].$ | Мопг78А0 |
| 3.44.3 | CCl_4 | 4.25×10^{5} | 4.0×10^{-3} | rt | Od-15 | S = self. k derived using $k_d = *1.7 \times 10^3$ s ⁻¹ [1.8.4]. | Bowe53F00 |
| 3.44.4 | CS ₂ | 1.4×10^6 | 3.6×10^{-3} | rt | Od-15 | S = self. k derived using $k_d = 5.0 \times 10^3 \text{ s}^{-1}$ [1.9]. | Bowe53F00 |
| 3.44.5 | CS ₂ | 1.9×10^{6} | 2.6×10^{-3} | rt | Ad-15 | S = DNT. k derived using $k_d = 5.0 \times 10^3 \text{ s}^{-1}$ | Foot72F0 |
| 3.44.6 | C_6H_6 | 9.5×10^4 | 4.2×10^{-1} | rt | Pa-15 | [1.9]. S = self. k derived using $k_d = *4.0 \times 10^4$ | Bowe.55F0 |
| 3.44.7 | C_6H_6 | 7.0×10^4 | 5.7×10^{-1} | rt | Ad-15 | s ⁻¹ [1.32.9]. S = self. k derived using $k_d = *4.0 \times 10^4$ | Livi.59F00 |
| 3.44.8 | C_6H_6 | 8.5×10^{5} | 4.7×10^{-2} | rt | Ad-15 | using $k_{\rm d} = *4.0 \times 10^4$ | Foot72F0 |
| .44.9 | C ₆ H ₆ | 1.6 × 10 ⁵ | $(2.7 \pm 0.5) \times 10^{-1}$ | 25 | A'd-20 | s^{-1} [1.32.9]. 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]. | Stev74F3 |
| 3.44.10 | C₀H₅Br | 1.1×10^{5} | 1.2×10^{-1} | rt | Ad-15 | S = self. k derived $u \sin g k_d = 1.3 \times 10^4 \text{ s}^{-1}$ [1.34]. | Livi.59F00 |
| 3.44.11 | CS ₂ /C ₆ H ₆ (99:1) Mole % | 3.3 × 10 ⁵ (est) | 1.5×10^{-2} | rt | Od-15 | S = self. k estimated using $k_d = 5.0 \times 10^3 \text{ s}^{-1}$ | Bowe53F0 |
| 3.44.12 | CS ₂ /C ₆ H ₆ (95:5) Mole % | 1.6×10^{5} (est) | 3.8×10^{-2} | rt | Od-15 | (calc). S = self. k estimated using $k_d = 6.2 \times 10^3 \text{ s}^{-1}$ | Bowe53F0 |
| 3.44.13 | CS_2/C_6H_6 (90:10) | 1.2×10^{5} (est) | 6.2×10^{-2} | rt | Od-15 | (calc). S = self. k estimated using $k_d = 7.5 \times 10^3 \text{ s}^{-1}$ | Bowe53F0 |
| 3.44.14 | Mole % CS ₂ /C ₆ H ₆ (96:4) | 2.4×10^{5} (est) | 2.7×10^{-2} | rt | Ad-15 | (calc). $S = DNT$. k estimated using $k_d = 6.4 \times 10^3 \text{ s}^{-1}$ | Foot72F0 |
| 3.44.15 | Mole % CS ₂ /C ₆ H ₆ (93:7) | 1.4×10^{5} (est) | 5.2×10^{-2} | rt | Ad-15 | (calc). $S = DNT$. k estimated using $k_d = 7.5 \times 10^3 \text{ s}^{-1}$ | Foot72F0 |
| 3.44.16 | Mole % CS ₂ /C ₆ H ₆ (75:25) | 1.5×10^5 (est) | 9.4×10^{-2} | rt | Ad-15 | using $k_{\rm d} = 1.4 \times 10^4 {\rm s}^{-1}$ | Foot72F0 |
| 3.44.17 | Mole % CS ₂ /C ₆ H ₆ (50:50) Mole % | 3.0×10^5 (est) | 7.7×10^{-2} | rt | Ad-15 | (calc). S = TPP. k estimated using $k_d = 2.3 \times 10^4 \text{s}^{-1}$ (calc). | Foot72F0 |
| | For more re | elative rates see | 3.41, 3.60, 3.64. | | | | |

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

| No. S | Substrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | <i>t</i> /°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 $k_d = *1.0 \times 10^4$ s ⁻¹ [1.5.3]. | Bowe53F004 |
| 3.45.1 | [24] 24] | CCl₄ | 4.1×10^{5} | 4.1×10^{-3} | rt | Od-15 | S = self. k derived using $k_d = *1.7 \times 10^3$ 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 $k_d = 5.0 \times 10^3 \text{ s}^{-1}$ [1.9]. | Bowe53F004 |
| 3.46 | 9-chloro- anthracene $[R_9 = -C1]$ | CHCl ₃ | 4.2×10^{5} | 2.4×10^{-2} | rt | Od-15 | S = self. k derived using $k_d = *1.0 \times 10^4$ s ⁻¹ [1.5.3]. | Bowe53F00 |
| 3.46.1 | [149 — -01] | CCl ₄ | 5.3×10^5 | 3.2×10^{-3} | rt | Od-15 | S = self. k derived using $k_d = *1.7 \times 10^3$ s ⁻¹ [1.8.4]. | Bowe53F00 |
| 3.46.2 | | CS ₂ | 1.7×10^{6} | 3.0×10^{-3} | rt | Od-15 | S = self. k derived using $k_d = 5.0 \times 10^3 \text{ s}^{-1}$ [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 $k_d = *1.0 \times 10^4$ s ⁻¹ [1.5.3]. | Bowe53F004 |
| 3.47.1 | [14] | CHCl ₃ | $(8.1 \pm 1.5) \times 10^6$ | · | rt | A'd-33 | S = A' = Rub. k derived using $k_r^{A'} = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3] and $k_d = 1.67 \times 10^4 \text{ s}^{-1}$ [1.5]. | Monr78A00 |
| 3.47.2 | | CCl ₄ | 5.2×10^5 | 3.3×10^{-3} | rt | Od-15 | S = self. k derived using $k_d = *1.7 \times 10^3$ s ⁻¹ [1.8.4]. | Bowe53F00 |
| 3.47.3 | | C ₆ H 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]. | Stev74F31 |
| 3.48 | 9-methoxy- anthracene $[R_9 = -OMe]$ | C ₆ H ₆ | $k_{\rm r}=2.5\times10^6$ | | 25 | Ad-17 A'd | S = A' = Tetr. Measured $(k_r/k_r^{A'}) = 0.21$. k_r derived using $k_r^{A'} = *1.2 \times 10^7 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [A3.13]. | Stev74F31 |
| 3.49 | 1-anthracene- sulfonate ion $[R_1 = -SO_3^-]$ | H ₂ O | 5.0 × 10 ⁸ | | 28 | P'a-23 | S = self. Q = NaN ₃ , A' = KI, P' = I_3^- . k derived using $k_d = 5.0 \times 10^5$ s ⁻¹ [I.I] and $k_Q = 2.2 \times 10^8$ dm ³ mol ⁻¹ s ⁻¹ [12.9.6]. | Roha.77F07 |
| 3.49.1 | | H ₂ O | 5.4×10^7 | 9.2×10^{-3} | 30 | Ad-15 | S = self. k derived using $k_d = 5.0 \times 10^5$ s ⁻¹ [1.1]. | Gupt78A2* |
| .50 | 2-anthracenesulfonate ion $[R_2 = -SO_3^-]$ | H ₂ O | 3.0×10^{8} | | 28 | P'a-23 | S = self. Q = NaN ₃ , A' = KI, P' = I_3 . k derived using $k_d = 5.0 \times 10^5$ s ⁻¹ [1.1] and $k_Q =$ 2.2 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ [12.9.6]. | Roha.77F07 |
| 3.50.1 | | H_2O | 4.5×10^7 | 1.1×10^{-2} | 30 | Ad-15 | S = self. k derived using $k_d = 5.0 \times 10^5$ s ⁻¹ [1.1]. | Gupt78A2 |
| 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 $k_d = *1.0 \times 10^4$ s ⁻¹ [1.5.3]. | Bowe53F00 |

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

| No. S | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /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]. | Bowe53F00 |
| 3.51.2 | | CS ₂ | 6.0×10^{6} | 8.4 × 10 ⁻⁴ | rt | Od-15 | S = self. k derived using $k_d = 5.0 \times 10^3 \text{ s}^{-1}$ [1.9]. | Bowe53F004 |
| 3.51.3 | | C ₆ H 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 $k_d =$ | Stev74F312 |
| 3.52 | 9,10-dichloro- anthracene $[R_9 = R_{10} = -Cl]$ | CHCl ₃ | 1.7×10^5 | 6.0×10^{-2} | rt | Od-15 | 4.2 × 10 ⁴ s ⁻¹ [1.32]. S = self. k derived using $k_d = *1.0 \times 10^4$ | Bowe53F00 |
| 3.52.1 | $K_{0} = K_{0} = -C_{0}$ | CCl ₄ | 1.7×10^5 | 1.0×10^{-2} | rt | Od-15 | s ⁻¹ [1.5.3]. S = self. k derived using $k_d = *1.7 \times 10^3$ | Bowe53F00 |
| 3.52.2 | | CS ₂ | 2.9×10^5 | 1.7×10^{-2} | rt | Od-15 | s^{-1} [1.8.4]. S = self. k derived $using k_d = 5.0 \times 10^3 s^{-1}$ | Bowe53F004 |
| 3.53 | 9,10-dimethyl- anthracene (DMA) $[R_9 = R_{10} = -Me]$ | H ₂ O | 9.1×10^{8} | 5.5 × 10 ⁻⁴ | 25 | Ad-15 | [1.9]. S = Eos. k derived $using k_d = 5.0 \times 10^5$ s^{-1} [1.1]. S and A solubilized in DTAC micelles. | Usui78F06 |
| 3.53.1 | | H ₂ O | 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 | Usui78F06 |
| 3.53.2 | | D ₂ O | 7.4×10^{8} *4.6 × 10 ⁸ | 6.8 × 10 ⁻⁵ | 25 | Ad-15 | micelles. S = MB. k derived using $k_d = 5.0 \times 10^4$ (*3.1 × 10 ⁴) s ⁻¹ [1.2.3]. A solubilized in DTAC | Usui78F06 |
| 3.53.3 | | МеОН | 2.4×10^{7} *1.25 × 10 ⁷ | $(8.0 \pm 1.5) \times 10^{-3}$ | 24 | Ad-15 | micelles. S = self. k derived using $k_d = 1.4 \times 10^5$ (*1.0 × 10 ⁵) s ⁻¹ [1.3]. | Stev.74F207 |
| 3.53,4 | | МеОН | 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 × 10 ⁵) s ⁻¹ [1.3]. Error is a 95% confidence line | Beth.77F113 |
| 3.53.5 | | CHCl ₃ | $k_{\rm r} = 2.7 \times 10^7$ *1.6×10 ⁷ | | 24 | Ad-17 A'd | S = A' = Rub. Measured $(k_r/k_r^{A'}) = 0.643. k_r$ derived using $k_r^{A'} = 4.2 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ | nit. Stev.74F207 |
| 3.53.6 | | CHCl ₃ | 9.3×10^{7} *5.6 × 10^{7} | $(1.8 \pm 0.7) \times 10^{-4}$ | rt | Ad-15 | [A3.14]. S = MB. k derived using $k_d = 1.67 \times 10^4$ (*1.0 × 10 ⁴) s ⁻¹ [1.5]. Error is a | Beth.77F113 |
| 3.53.7 | | CCl ₄ | $k_{\rm r} = 7.0 \times 10^6$ *2.1 × 10 ⁷ | | 24 | Ad-17 A'd | 95% confidence limit. $S = A' = Rub$. Measured $(k_r/k_r^A) = 0.5$. k_r derived using $k_r^A = 1.4 \times 10^7$ (*4.2 × 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 /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|--|--|---------------------------------------|----------|--------------|---|-------------|
| 3.53.8 | CS ₂ | $k_{\rm r} = 1.3 \times 10^7$ *2.1 × 10 ⁷ | | 24 | Ad-17 A'd | $S = A' = Rub$. Measured $(k_r/k_r^{A'}) = 0.5$. k_r derived using $k_r^{A'} = 2.5 \times 10^7 (*4.2 \times 10^7)$ dm ³ mol ⁻¹ s ⁻¹ [43.14]. | Stev.74F20 |
| 3.53.9 | CH ₃ CN | 1.7×10^8 *1.3 × 10 ⁸ | $(2.0 \pm 0.4) \times 10^{-4}$ | rt | Ad-15 | min for (13.74) . $S = MB$. 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.77F11 |
| 3.53.10 | EtOH | 1.2×10^7 | $(7.2 \pm 1.4) \times 10^{-3}$ | 24 | Ad-15 | | Stev.74F207 |
| 3.53.11 | EtOH | 3.9×10^7 | 2.1×10^{-3} | 25 | Ad-15 | | Usui.78F06 |
| 3.53.12 | EtOH | 4.4×10^7 | 1.9 × 10 ⁻³ | 25 | Ad-15 | | Usui.78F06 |
| 3.53.13 | CCl ₂ F- CClF ₂ | 4.2×10^{5} $k_{\rm r} = 2.8 \times 10^{5}$ | 1.1×10^{-5} | 25 | Ad-34 | | Evan.76F41 |
| | | $k_{\rm q}=1.4\times10^{\rm 5}$ | | | | 0.5. k , k_r , and k_q derived using $k_d = 4.7 \times 10^2 \text{ s}^{-1}$ ([1(a).2];[1(a).2.1]) ^a . | |
| 3.53.14 | CCl ₂ F- CClF ₂ | 5.2×10^{5} $k_{\rm r} = 2.9 \times 10^{5}$ | 9.1 × 10 ⁻⁵ | 25 | Ad-34 | ${}^{1}O_{2}$ * from He/Ne laser (632.8 nm). Measured $(k_{q}/k_{r}) = 0.76. k$, | Evan.76F41 |
| 3.53.15 | C5H5N | $k_{\rm q} = 2.2 \times 10^5$ 3.0×10^7 | | rt | Ad-20 | Measured $(k_{A'}/k) = 1.0$. k derived using $k_{A'} = *3.0 \times 10^7 \text{ dm}^3$ | Wils66F041 |
| 3.53.16 | C ₅ H ₅ N | 4.2×10^7 | 1.4×10^{-3} | 12 | Pa-20 | mol ⁻¹ s ⁻¹ [A3.2]. S = thionine, A' = TME. k derived using | Kram.73F20 |
| 3.53.17 | C ₅ H ₅ N | 5.9×10^{7} | 1.0×10^{-3} | 12 | Pa-20 | $k_{\rm d} = 5.9 \times 10^4 {\rm s}^{-1} [\it{I}.29.I].$ S = MB, A' = TME. k derived using $k_{\rm d} = 5.9 \times 10^4 {\rm s}^{-1} [\it{I}.29.I].$ | Kram.73F20 |
| 3.53.18 | C ₅ H ₅ N | 4.2×10^7 | 1.4×10^{-3} | 12 | Pa-20 | $k_d = 5.9 \times 10^{-8} \cdot [1.29.1].$ S = self, A' = TME. $k \text{ derived using } k_d = 5.9 \times 10^4 \text{ s}^{-1} [1.29.1].$ | Kram.73F20 |
| 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 $k_d = 5.9 \times 10^4 \text{ s}^{-1} [1.30].$ | Stev.74F207 |
| 3.53.20 | C ₆ H 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]. | Stev.69F388 |
| 3.53.21 | C ₆ H ₆ | 1.3×10^8 | 3.0×10^{-4} | 25 | Ad-15 | k is a mean for both S. S = Rub. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Alga.70E07 |
| 3.53.22 | C ₆ H ₆ | 1.3×10^{8} | 3.0×10^{-4} | 25 | Ad-15 | S = self. k derived using $k_d = *4.0 \times 10^4$ 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 /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|---|---|---------------------------------------|----------|---------------|--|-------------|
| 3.53.2 | 3 | C ₆ H ₆ | 1.3 × 10 ⁸ | 3.0 × 10 ⁻⁴ | 25 | Ad-15 | S = Tetr. k derived using $k_d = *4.0 \times 10^4$ $e^{-1} (1.32.0)$ | Alga.70E07 |
| 3.53.2 | 4 | C ₆ H ₆ | 2.1×10^7 | $(2.0 \pm 0.5) \times 10^{-3}$ | 25 | Ad-15 | s ⁻¹ [1.32.9]. S = self. k derived using $k_d = 4.2 \times 10^4 \text{ s}^{-1}$ [1.32]. | Stev74F31 |
| 3.53.2 | 5 | C ₆ H 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]. | Stev76F42 |
| 3.53.2 | | C ₆ H ₅ Br | 3.0×10^7 | | rt | Ad-20 | S = MB, A' = TME. Measured (k_A/k) = 1.0. k derived using $k_{A'} = *3.0 \times 10^7 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [A3.2]. | Wils66F041 |
| | | For more | relative rates see | 3.62.5, 3.63.16, 9.1.2, 11.31.4. | 9.1.4–5 | , 9.4.2, 9.6. | 2, 9.6.4, | |
| 3.54 | 9,10-dimethoxy- anthracene $[R_9 = R_{10} = -OMe$ | C ₆ H ₆ e] | $k_{\rm r}=1.4\times10^7$ | | 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]. | Stev74F31 |
| 3.55 | 1,5-anthracene- disulfonate ion $[R_1 = R_5 = -SO_3^-]$ | H ₂ O | < 10 ⁷ (est) | | 28 | P'a-23 | | Roha.77F07 |
| 3.55.1 | | H ₂ O | $7.0 	imes 10^6$ | 7.0×10^{-2} | 30 | Ad-15 | | Gupt78A2 |
| 3.56 | 9,10-diphenyl- anthracene $[R_9 = R_{10} = -Ph]$ | CHCl ₃ | $2.5 	imes 10^6$ | 4.0×10^{-3} | rt | Od-15 | | Bowe53F00 |
| 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [3.63.3] and k_d = 1.67 × 10 ⁴ s ⁻¹ [1.5]. | Monr78A00 |
| 3.56.2 | | CCl ₄ | 2.8×10^6 | 6.0×10^{-4} | rt | Od-15 | | Bowe53F00 |
| 3.56.3 | | CS ₂ | 1.6×10^6 | 3.2×10^{-3} | rt | Od-15 | | Bowe53F00 |
| 3.56.4 | | CFCl ₂ - CF ₂ Cl | $k_{\rm r} = 4.0 \times 10^{\rm 5}$ (est) | | rt | Ad-36 | $^{1}O_{2}^{*}$ 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 | Math.70F38 |
| 2 56 5 | | CHN | 5.4 > 100 | | | | value of $k_{O_2} = 1.3 \times 10^3$ dm ³ mol ⁻¹ s ⁻¹). | |
| 3.56.5 | | C ₅ H ₅ N | 5.4 × 10 ⁶ | | rt | Ad-20 | S = self. A' = TME. Measured (k_A/k) = 5.6. k derived using $k_{A'}$ = *3.0 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [A3.2]. | Wils66F014 |
| 3.56.6 | | C ₆ H ₆ | 7.0×10^{5} | 5.7×10^{-2} | rt | Ad-15 | | Bowe.55F00 |
| 3.56.7 | | C ₆ H 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. S | Substrate (A) | Solvent | $\frac{k}{\text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|--|-------------------------------|---|---------------------------------------|----------|--------------|--|-------------|
| 3.56.8 | | C ₆ H 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 ₆ H ₆ | 1.0×10^{6} | $(4.0 \pm 0.5) \times 10^{-2}$ | 25 | Ad-15 | S = self. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Stev.72F196 |
| 3.56.10 |) | C ₆ H 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 $k_d = 4.2 \times 10^4$ s ⁻¹ [1.32]. | Stev74F312 |
| 3.57 | 1-chloro-9,10- diphenylanthracene $[R_1 = -Cl, R_9 = R_{10} = -Ph]$ | CHCl ₃ | relative rates see $(2.0 \pm 0.5) \times 10^6$ | 4.28.13, 11.14.3. | 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]. | Monr78A00 |
| 3.58 | 1-methylamino- 9,10-diphenyl- anthracene {R ₁ = -NHCH ₃ , | C ₆ H ₆ | 3.3×10^8 | $(1.2 \pm 0.2) \times 10^{-4}$ | 25 | Ad-15 | | Stev.75F558 |
| 3.59 | $R_9 = R_{10} = -Ph$] 1,4-dimethoxy- 9,10-diphenyl- anthracene $[R_1 = R_4 = -OMe,$ $R_9 = R_{10} = -Ph$] | CHCl ₃ | $(3.2 \pm 0.5) \times 10^8$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'}$ = $5.3 \times 10^7 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3] and k_{d} = $1.67 \times 10^4 \text{ s}^{-1}$ [1.5]. | Monr78A00: |
| 3.60 | 1,2-benz- anthracene | C ₆ H ₆ | $k_{\rm r}=4.8\times10^4$ | | 25 | Ad-17 A'd | S = A' = An. Measured $(k_r/k_r^{A'}) = 0.30. k_r$ derived using $k_r^{A'} = 1.6 \times 10^5 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [3.44.9]. | Stev74F312 |
| 3.61 | 9,10-dimethyl- 1,2-benzanthracene | H ₂ O | 1.1×10^{10} | 4.0 × 10 ⁻⁵ | rt | Ad-15 | S = MB. k derived using $k_d = *4.4 \times 10^5$ s ⁻¹ [1.13]. A solubilized in CTAB micelles. | Gree.78N00 |
| 3.61.1 | ĊH₃ | C ₆ H 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]. | Stev.69F388 |
| 3.61.2 | | C ₆ H ₆ | 5.6×10^7 | 7.1×10^{-4} | 25 | Ad-15 | using $k_{\rm d} = *4.0 \times 10^4$ | Alga70E07 |
| 3.61.3 | | C ₆ H ₆ | 5.6×10^{7} | 7.1×10^{-4} | 25 | Ad-15 | using $k_{\rm d} = *4.0 \times 10^4$ | Alga70E07 |
| 3.61.4 | | C ₆ H ₆ | 4.8×10^7 | 8.3×10^{-4} | 25 | Ad-15 | using $k_{\rm d} = *4.0 \times 10^4$ | Alga70E07 |
| 3.61.5 | | C ₆ H ₆ | $k_{\rm r}=1.4\times10^7$ | | 25 | Ad-17 A'd | s ⁻¹ [1.32.9]. S = A' = Rub. Measured $(k_r/k_r^{A'}) = 0.33$. k_r derived using $k_r^{A'} = 4.2 \times 10^7 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [3.63.18]. | Stev74F312 |

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

| No. S | Substrate (A) | Solvent | /dm³ mol-1 s-1 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|--|--|---|----------|--------------|--|-------------|
| 3.61.6 | | C ₆ H ₆ | 2.5×10^7 | 1.6 × 10 ⁻³ | 25 | Ad-? | S = self. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Stev.76F422 |
| 3.62 | tetracene (2,3-benzanthra- cene) | For more re CH ₂ Cl ₂ | elative rates see $3.0 	imes 10^7$ | $3.62.6, 3.63.17.$ 4.0×10^{-4} | rt | Ad-14 | S = self. k derived using $k_d = *1.2 \times 10^4$ s ⁻¹ [1.4.2]. | Byst.75F654 |
| | | | | | | | | |
| 3.62.1 | | CCl ₄ | $(5.0 \pm 1.5) \times 10^6$ | | rt | Ld-13 | $k_{\rm d} = 3.6 \times 10^1 {\rm s}^{-1}$ | Kras79A010 |
| 3.62.2 | | CCl ₄ | $k_{\rm r}=5\times10^6$ | | rt | Ad-27 28 | [1.8.3]. S = ? k_r derived using $k_A = 5.0 \times 10^6$ dm ³ mol ⁻¹ s ⁻¹ 13.63 H | Kras79A016 |
| 3.62.3 | | n-BuOH | 5.2×10^8 | 1.0 × 10 ⁻⁴ | 20 | Ad-15 | dm ³ mol ⁻¹ s ⁻¹ [3.62.1]. S = MB. k derived using $k_d = 5.2 \times 10^4$ s ⁻¹ [1.24]. | Snya78A2 |
| 3.62.4 | | C ₆ H ₆ | 2.4×10^7 | 1.7×10^{-3} | 25 | Ad-15 | | Alga.70E07 |
| 3.62.5 | | C ₆ H ₆ | $k_{\rm r}=8.5\times10^6$ | | 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 | Alga.70E07 |
| 3.62.6 | | C ₆ H ₆ | $k_r = 1.5 \times 10^7$ | | 25 | Pa–17 P'a | mol ⁻¹ s ⁻¹ [A3.10]. 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.70E07 |
| .62.7 | | C ₆ H ₆ | $k_{\rm r}=1.2\times10^7$ | | 25 | Ad-17 A'd | S = A' = rub. Measured $(k_r/k_r^{A'}) = 0.29$. k_r derived using $k_r^{A'} = 4.2 \times 10^7$ dm ³ mol ⁻¹ s ⁻¹ [3.63.18]. | Stev74F31 |
| .62.8 | | C ₆ H ₆ | 1.7×10^7 | 2.4×10^{-3} | 25 | Ad-? | S = self. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Stev.76F42 |
| 3.63 | 5,6,11,12-tetra- phenylnaphthacene (Rub) | MeOH | relative rates see 3.1×10^7 *2.2 \times 107 | $3.48, 6.33.3, 7.5.1.$ $(4.5 \pm 0.9) \times 10^{-3}$ | 24 | Ad-15 | S = self. k derived using $k_d = 1.4 \times 10^5$ (*1.0 × 10 ⁴) s ⁻¹ [1.3]. | Stev.74F20 |
| | C ₆ H ₅ C ₆ H ₅ | | | | | | | |
| 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.74F20 |
| 3.63.2 | | CHCl ₃ | 5.9×10^{7} *3.4 × 10 ⁷ | $(2.9 \pm 1.0) \times 10^{-4}$ | 25 | Ad-15 | | Brau.75E22 |
| 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. | Monr77F48 |

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

| No. Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|---|--|---------------------------------------|----------|--------------|--|-------------|
| 3.63.4 | CCl₄ | 1.4 × 10 ⁷ | $(1.0 \pm 0.5) \times 10^{-4}$ | 24 | Ad-15 | S = self. k derived using $k_d = 1.4 \times 10^3 \text{ s}^{-1}$ [1.8]. | Stev.74F207 |
| 3.63.5 | CCI ₄ | 2.3×10^7 | $(6.0 \pm 3.0) \times 10^{-5}$ | 25 | Ad-15 | | Brau.75E223 |
| 3.63.6 | CS_2 | 2.5×10^7 | $(2.0 \pm 0.5) \times 10^{-4}$ | 24 | Ad-15 | • • | Stev.74F207 |
| 3.63.7 | CS ₂ | 5.6×10^7 | $(9.0 \pm 3.0) \times 10^{-5}$ | 25 | Ad-15 | | 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 $k_d = 8.3 \times 10^4 \text{s}^{-1}$ [1.10]. | Stev.74F207 |
| 3.63.9 | CFCl ₂ - CF ₂ Cl | $k_{\rm r} = 3.2 \times 10^6 $ (est) | | rt · | Ad-36 | $^{1}O_{2}$ * directly from CW Nd-YAG laser (1065 nm). Measured $(k_{r}/k_{O_{2}}[O_{2}] =$ 800. k_{r} estimated using $k_{O_{2}}[O_{2}] =$ 4×10^{3} s ⁻¹ (based on gas phase value of $k_{O_{2}} =$ | Math.70F38 |
| 3.63.10 | C₅H₅N | 7.1×10^7 | | rt | Ad-20 | 1.3 × 10 ³ dm ³ mol ⁻¹ s ⁻¹). S = MB, A' = TME. Measured (k_A/k) = 4.2 × 10 ⁻¹ . k derived using $k_{A'}$ = *3.0 × 10 ⁷ dm ³ | Wils66F041 |
| 3.63.11 | C ₅ H ₅ N | 6.4×10^7 | | rt | Ad-20 | mol ⁻¹ s ⁻¹ [A3.2]. S = self, A' = TME. Measured $(k_A/k) = 4.7 \times 10^{-1}$. k derived using $k_{A'} = *3.0 \times 10^7$ dm ³ | Wils66F041 |
| 3.63.12 | C_6H_{12} | 1.5×10^7 | $(4.0 \pm 0.8) \times 10^{-3}$ | 24 | Ad-15 | mol ⁻¹ s ⁻¹ [A3.2]. S = self. k derived using $k_d = 5.9 \times 10^4 \text{ s}^{-1}$ | Stev.74F207 |
| 3.63.13 | C_6H_6 | 1.3×10^{10} | 3×10^{-6} | rt | Ad-15 | [1.30]. S = self. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Bowe34F00 |
| 3.63.14 | C ₆ H ₆ | 2.4×10^7 | 1.7×10^{-3} | rt | Ad-15 | | Bowe55F00 |
| 3.63.15 | C ₆ H ₆ | 1.3×10^{8} | 3.0×10^{-4} | 25 | Ad-15 | | Alga.70E079 |
| 3.63.16 | C_6H_6 | $k_{\rm r}=4.7\times10^7$ | | 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 ₆ H ₆ | $k_{\rm r}=9.0\times10^7$ | | 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 ₆ H ₆ | 4.2×10^7 | $(1.0 \pm 0.1) \times 10^{-3}$ | 25 | Ad-15 | _ | Stev74F312 |

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

| No. S | ubstrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|---|---|--|--|----------|---------------|--|-------------|
| 3.63.19 | | C ₆ H ₆ | 4.7 × 10 ⁷ | $(8.5 \pm 2.0) \times 10^{-4}$ | 25 | Ad-23 | S = self, A' = lipoic acid. k derived using $k_d = *4.0 \times 10^4 \text{ s}^{-1}$ [1.32.9]. | Stev74F641 |
| 3.63.20 | | C₀H₀ | $k_{\rm r}=4.3\times10^7$ | | 25 | Ad-17 A'd | (h225). 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 ¹ O ₂ * interacting with A' causes the destruction of 2 molecules of A'. | Stev74F641 |
| 3.63.21 | | C ₆ H ₆ | 4.7×10^7 | $(9.0 \pm 2.5) \times 10^{-4}$ | 25 | Ad-15 | | Brau.75E223 |
| 3.63.22 | | C ₆ H ₆ | 4.0×10^7 | 1.0×10^{-3} | 25 | Ad-? | S = self. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Stev.76F422 |
| 3.63.23 | | C ₆ H ₅ Br | 1.6×10^7 | $(8.0 \pm 2.0) \times 10^{-4}$ | 24 | Ad-15 | S = self. k derived using $k_d = 1.3 \times 10^4 \text{ s}^{-1}$ [1.34]. | Stev.74F207 |
| 3.63.24 | | 1,2,3- C ₆ H ₃ Cl ₃ | 5.0×10^{7} (est) | $(4.0 \pm 1.5) \times 10^{-4}$ | 25 | Ad-15 | | Brau.75E223 |
| 3.63.25 | | C ₆ H ₅ CH ₃ | 4.4×10^7 | $(9.1 \pm 2.5) \times 10^{-4}$ | 25 | Ad-15 | S = self. k derived using $k_d = *4.0 \times 10^4 \text{ s}^{-1}$ [1.36]. | Brau.75E223 |
| | | For more r | elative rates see | 3.53.5, 3.53.7–8, 3.54, 14.32.11, 14.32.14, 14 | | , 3.62.7, 5.3 | | |
| 3.64 | 1,2,5,6-dibenz- anthracene | C ₆ H ₁₂ | $k_{\rm r}=9.5\times10^3$ | 17.32.11, 17.32.17, 17 | 25 | Ad-17 A'd | S = A' = An. Measured $(k_r/k_r^{A'}) = 0.59$. k_r derived using $k_r^{A'} = 1.6 \times 10^5 \text{ dm}^3 \text{ mol}^{-1}$ s^{-1} [3.44.9]. | Stev74F312 |
| 3.65 | pentacene | C₀H₀ | $k_{\rm r} = 4.2 \times 10^9$ *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 [43.17]. | Stev74F312 |
| 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 $k_d = 1.7 \times 10^4 (*1.0 \times 10^4)$ s ⁻¹ [1.5]. | Wage.76F57 |
| | | | | | | | | |
| 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 $k_d = 1.7 \times 10^3 \text{ s}^{-1}$ [1.8.4]. | Wage.76F57 |

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 | $\beta (k_d/k)$ /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 $k_d = 5.0 \times 10^3 \text{ s}^{-1}$ [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]. | Drew77F17 |
| 3.66.4 | C ₆ H ₆ | 7.0×10^7 | $(6.0 \pm 2.0) \times 10^{-4}$ | 25 | Ad-15 | S = self. k derived using $k_d = 4.2 \times 10^4 \text{ s}^{-1}$ [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]. | Drew77F17 |
| 3.66.6 | C ₆ H ₅ CH 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 ₆ H ₃ Cl ₃ | $\begin{array}{c} 2.4 \times 10^7 \\ \text{(est)} \end{array}$ | $(5.5 \pm 1.5) \times 10^{-4}$ | 25 | Ad-15 | S = self. k estimated using $k_a(C_6H_5Br) = 1.3 \times 10^4 \text{ s}^{-1} [1.34]$. | Wage.76F570 |

^{*}This value of $k_{\rm d}$ is an average of the $k_{\rm d}$ 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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|---|---|--|---|---------------------------------|--------|--|-------------|
| | | | | all rate constant unless <i>k</i> is specified; <i>k</i> is the rat | | | | |
| 4.1 | 2,6-di- t -butyl- phenol OH $(CH_3)_3C$ $(CH_3)_3$ | MeOH | 1.01×10^6 | 1.15×10^{-1} | rt | | S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5 \text{ s}^{-1}$ $([1.3];[1.3.2];[1.3.3])^a$. | Thom.78A17 |
| 4.1.1 | | | 1.7×10^{6} | | 20 | A'd-23 | S = MB, A' = Tetr. k derived using $k_{A'}$ = $5.2 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.62.3] and k_d = $5.2 \times 10^4 \text{ s}^{-1}$ [1.24]. | Snya78A26 |
| 4.1.2 | | C ₆ H ₆ | 3.2×10^4 | | rt | P'a-20 | S = ZnTPP, A' = 2M2P. Measured $(k[A] + k_d)/k_{A'} =$ $6.17 \times 10^{-2} \text{ mol dm}^{-3} \text{ at}$ $[A] = 2.2 \times 10^{-1} \text{ mol dm}^{-3}$. k derived using $\beta_{A'} = 5.3 \times 10^{-2} \text{ mol dm}^{-3}$ $[2.40.23]$ and $k_d =$ $4.17 \times 10^4 \text{ s}^{-1} [1.32]$. | Thom.78A17 |
| 4.2 | 4-(1,1,3,3-tetra- methylbutyl)- phenylsalicylate | i-octane | relative rates see < 1 × 10 ⁶ (est) | 2.101, 2.101.1. | · rt | A'd-23 | S = A' = Rub. No measurable effect. | Carl73P066 |
| | C000C(CH ₃) ₂ CH ₂ C | C(CH ₃) ₃ | | | | | | |
| 4.3 | 2-hydroxy-4- octyloxybenzo- phenone | C ₆ H ₅ Br | < 1 × 10 ⁶ (est) | | 0 | A'd-33 | ${}^{1}O_{2}^{*}$ from microwave discharge, $A' = Rub$. No measurable effect. | Guil.73F333 |
| 4.3.1 | | CCl ₄ | 1.0 × 104 | | | | | |
| | | /CHCl ₃ (9:1) v:v | 1.0×10^4 (est) | | rt | A'd-23 | S = A' = Rub. Measured $k/(k_A\{A'] + k_d) = 10.0 \text{ dm}^3 \text{ mol}^{-1} \text{ at}$ [A'] = $5 \times 10^{-6} \text{ mol dm}^{-3}$. $k \text{ estimated using } k_{A'} = 7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 1.43 \times 10^3 \text{ s}^{-1}$ [1.8]. | Hrdl74F64: |
| 4.4 | 2-hydroxy-4- dodecyloxybenzo- phenone | i-octane | $ < 1 \times 10^6 $ (est) | | rt | A'd-23 | S = A' = Rub. No measurable effect. | Carl73P066 |
| | O O (CH ₂ (C | сн ⁵) ¹⁰ сн ³) | | | | | | |
| 4.4.1 | | CCl₄ /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 : | | | |
| | | | | (CH ³) ³ C OH | (CH ₃) ₃ | | | |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|--|-------------------------------|---|---------------------------------------|----------|--------------|--|-------------|
| 4.5 | 4-bromo-2,6-di- t-butylphenol [R ₄ = -Br] | МеОН | 8.41 × 10 ⁵ | 1.38 × 10 ⁻¹ | rt | A'd-16 | S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5 \text{ s}^{-1}$ | Thom.78A171 |
| 4.5.1 | | n-BuOH | 1.5×10^6 | | 20 | A'd-23 | ([1.3];[1.3.2];[1.3.3]) ^a . S = MB, A' = Tetr. k derived using $k_{A'}$ = 5.2 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ [3.62.3] and k_{d} = | Syna78A266 |
| 4.6 | 4-chloro-2,6-di- t-butylphenol [R ₄ = -Cl] | n-BuOH | 3.2×10^{6} | | 20 | A'd-23 | 5.2 × 10 ⁴ s ⁻¹ [1.24]. S = MB, A' = Tetr. k derived using k_A = 5.2 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ [3.62.3] and k_d = 5.2 × 10 ⁴ s ⁻¹ [1.24]. | Snya78A266 |
| 4.7 | 4-methyl-2,6- di- t -butylphenol [$R_4 = -Me$] | МеОН | 5.6×10^6 | 2.09×10^{-2} | rt | A'd-16 | S = MB, $A' = DPF$. k derived using $k_d = 1.16 \times 10^5 \text{ s}^{-1}$ $([1.3];[1.3.2];[1.3.3])^a$. | Thom.78A171 |
| 4.7.1 | | МеОН | 4.19×10^{6} | $(2.8 \pm 1.4) \times 10^{-2}$ | rt | Pa-15 | S = MB. k derived using $k_d = 1.16 \times 10^5 \text{ s}^{-1}$ $([1.3]; [1.3.2]; [1.3.3])^a$. | Thom.78A171 |
| 4.7.2 | | МеОН | $k_{\rm r} = 2.2 \times 10^5$ *2.9 × 10 ⁵ | | | Pa-17 P'a | S = MB, A' = 2M2P. Measured $(k_r/k_r^{A'}) = 0.357. k_r$ derived using $k_r^{A'} = 6.25 \times 10^5$ $(*8.1 \times 10^5) \text{ dm}^3 \text{ mol}^{-1}$ $s^{-1} [2.40.2, A3.3].$ | Thom.78A171 |
| 4.7.3 | i | EtOH | $< 1 \times 10^9$ (est) | | 0 | Od-23 | S = MB, A' = DMF. No measurable effect. | Dall72F518 |
| 4.7.4 | | n-BuOH | 7.6 x 10 ⁶ | | 20 | A'd-23 | S = MB, A' = Tetr. k derived using $k_{A'}$ = 5.2×10^8 dm ³ mol ⁻¹ s ⁻¹ [3.62.3] and k_d = 5.2×10^4 s ⁻¹ [1.24]. | Syna78A266 |
| 4.7.5 | i | C_6H_6 | 2.53×10^{6} | 1.65×10^{-2} | rt | A'd-16 | S = ZnTPP, A' = DPF. $k \text{ derived using } k_d = 4.17 \times 10^4 \text{ s}^{-1} [1.32].$ | 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 × 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 ₆ H 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 ₆ H ₆ | $k_{\rm r} = 1.2 \times 10^5$ *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 × 10 ⁵ (*8.1 × 10 ⁵) dm ³ mol ⁻¹ | Thom.78A171 |
| | | For more | relative rates see | 4.12. | | | s ⁻¹ [2.40.23, A3.3]. | |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|--|-------------------------------|--|---------------------------------------|----------|--------------|--|-------------|
| 4.8 | 4-methoxy-2,6-di- t -butylphenol [$R_4 = -OCH_1$] | n-BuOH | 2.6×10^7 | | 20 | Ad-15 | S = MB. k derived using $k_d = 5.2 \times 10^4 \text{s}^{-1}$ | Snya78A266 |
| 4.8.1 | [14] = -00113] | n-BuOH | 2.7×10^7 | | 20 | A'd-23 | [1.24]. S = MB, A' = Tetr. k derived using $k_{A'}$ = $5.2 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.62.3] and k_d = $5.2 \times 10^4 \text{ s}^{-1}$ [1.24]. | Snya78A266 |
| 4.9 | 4-hydroxy-3,5- di- t -butyl benzyl alcohol [$R_4 = -CH_2OH$] | МеОН | 1.47×10^6 | 7.89×10^{-2} | rt | | S = MB, $A' = DPF$. k derived using $k_d = 1.16 \times 10^5 \text{ s}^{-1}$ $([1.3], [1.3.2], [1.3.3])^a$. | Thom.78A171 |
| 4.9.1 | | C ₆ H ₆ | 4.1×10^5 $*4.5 \times 10^5$ | | rt | P'a-19 | S = ZnTPP, A' = 2M2P. Measured (k/k_A) = 0.55. k derived using $k_{A'}$ = 7.5 × 10 ⁵ | Thom.78A171 |
| 4.10 | 4-acetyl-2,6-di- t-butylphenol $[R_4 = \text{-COCH}_3]$ | n-BuOH | 1.0 × 10 ⁶ | | 20 | A'd-23 | (*8.1 × 10 ⁵) dm ³ mol ⁻¹ s ⁻¹ [2.40.23, A3.3]. S = MB, A' = Tetr. k derived using $k_{A'}$ = 5.2 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ | Snya78A266 |
| 4.11 | methyl 3,5-di-t- | n-BuOH | 9.2 × 10 ⁵ | | 20 | A'd-23 | [3.62.3] and $k_d =$ 5.2 × 10 ⁴ s ⁻¹ [1.24]. S = MB, A' = Tetr. k | Snya78A266 |
| | butyl-4-hydroxy- benzoate $[R_4 = -COOCH_3]$ | | | | | | derived using $k_{A'} = 5.2 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.62.3] and $k_d = 5.2 \times 10^4 \text{ s}^{-1}$ [1.24]. | |
| 4.12 | 2,4,6-tri- t - butylphenol [$R_6 = -t$ -Bu] | МеОН | 3.41×10^6 | 3.40×10^{-2} | rt | A'd-16 | S = MB, $A' = DPF$. k derived using $k_d = 1.16 \times 10^5 \text{ s}^{-1}$ $([1.3]; [1.3.2]; [1.3.3])^a$. | Thom.78A171 |
| 4.12. | 1 | МеОН | $k_{\rm r} = 6.3 \times 10^4$ *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 × 10 ⁵ $(*2.9 \times 10^5)$ dm ³ mol ⁻¹ | Thom.78A171 |
| 4.12. | 2 | n-BuOH | 3.7×10^{6} | | 20 | A'd-23 | s ⁻¹ [4.7.2]. S = MB, A' = Tetr. k derived using $k_{A'}$ = 5.2 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ [3.62.3] and k_d = 5.2 × 10 ⁴ s ⁻¹ k 1.2 m | Snya78A266 |
| 4.12. | 3 | C ₆ H ₆ | 1.39 × 10 ⁶ | 3.0×10^{-2} | rt | A'd-16 | 5.2 × 10 ⁴ s ⁻¹ [1.24]. S = ZnTPP, A' = DPF. k derived using $k_d = 4.17 \times 10^4$ s ⁻¹ [1.32]. | Thom.78A171 |
| 4.12. | 4 | C ₆ H 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 × 10 ⁵ (*8.1 × 10 ⁵) dm ³ mol ⁻¹ s ⁻¹ [2.40.23, A3.3]. | Thom.78A171 |
| 4.13 | $\begin{aligned} &\text{4-}t\text{-butoxy-2,6-}\\ &\text{di-}t\text{-butylphenol}\\ &[\text{R}_4 = -\text{OC}(\text{CH}_3)_3] \end{aligned}$ | n-BuOH | 2.4×10^7 | | 20 | A'd-23 | S = MB, A' = Tetr. k derived using $k_{A'}$ = $5.2 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.62.3] and k_{d} = $5.2 \times 10^4 \text{ s}^{-1}$ [1.24]. | Syna78A266 |

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

| No. | Substrate (A) | Solvent | /dm³ mol-1 s-1 | $\beta (k_d/k)$ /mol dm ⁻³ | t ∕°C | Method | Comments | Ref. |
|--------|---|--|---|---------------------------------------|----------|--------------|--|-------------|
| 4.14 | 4-phenyl-2,6- di- t -butylphenol [$R_4 = -Ph$] | МеОН | 7.89 × 10 ⁶ | 1.47×10^{-2} | rt | A'd-16 | S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5 \text{ s}^{-1}$ $([1.3];[1.3.2];[1.3.3])^a$. | Thom.78A171 |
| 4.14.1 | | n-BuOH | 3.9×10^6 | | 20 | A'd-23 | S = MB, A' = Tetr. k derived using $k_{A'}$ = $5.2 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ $[3.62.3] \text{ and } k_{d}$ = $5.2 \times 10^4 \text{ s}^{-1} [1.24]$. | Snya78A266 |
| 4.15 | 4-benzyl-2,6-di- t -butylphenol [$\mathbf{R}_4 = -\mathbf{C}\mathbf{H}_2\mathbf{C}_6\mathbf{H}_5$] | МеОН | 3.76×10^6 | 3.08×10^{-2} | rt | A'd-16 | S = MB, A' = DPF. k derived using $k_0 = 1.16 \times 10^5 \text{ s}^{-1}$ $([1.3];[1.3.2];[1.3.3]^a$. | Thom.78A171 |
| 4.16 | 3-methoxy-4,6- di-t-butylphenol | MeOH(?) | $k_{\rm r}=2.1\times10^5$ | | 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]. | Sait70F454 |
| 4.16.1 | | MeOH(?) | $k_{\rm r}=2.0\times10^{\rm s}$ | | rt | Pa-17 P'a | $^{1}O_{2}$ * from H ₂ O ₂ /NaOCl, A' = TME. Measured $(k_{r}/k_{r}^{A'}) = 6.7 \times 10^{-3}$. k_{r} derived using $k_{r}^{A'} =$ *3.0 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [A3.2]. | Sait70F454 |
| 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. | Carl73P066 |
| | (CH ₃) ₃ C CH ₃ CH ₂ C-(CH ₃) ₃ | O(CH₂(CH₂)₁₆CH₃) | | | | | | |
| 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-butyl- phenyl 3,5-di-t- butyl-4-hydroxy- benzoate | | $\leq 1.0 \times 10^6$ (est) | | 0 | A'd-33 | ¹ O ₂ * from microwave discharge, A' = Rub. No measurable effect. | Guil.73F333 |
| | (CH ₃) ₃ C C(CH ₃) ₃ | C(CH ³) ³ | | / | | | | |
| 4.18.1 | | i-octane | $< 1.0 \times 10^{6}$ | | rt | A'd-23 | S = A' = Rub. No measurable effect. | Carl73P066 |
| 4.19 | 2-(2'-hydroxy-3'-chloro-5'-t-butyl-phenyl)benzo-triazole | CCl ₄ /CHCl ₃ (9:1) v:v | (est) 1.0 × 10 ⁴ (est) | | rt | A'd-23 | No measurable effect. $S = A' = Rub$. Measured $k/(k_A[A'] + k_d) = 10.0 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at $[A'] = 5 \times 10^{-6} \text{ mol}$ dm ⁻³ . k estimated using $k_{A'} = 7 \times 10^7$ dm ³ mol ⁻¹ s ⁻¹ and $k_d = 1.43 \times 10^3 \text{ s}^{-1}$ [1.8]. | Hrdl74F654 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|---|---|--|---------------------------------------|----------|--------|---|-------------|
| 4.20 | 2-(3',5'-di-t-butyl-2'-hydroxy-phenyl)-5-chloro-benzotriazole | C ₆ H ₅ Br | 2.6 × 10 ⁶ (est) | | 0 | A'd-33 | discharge, A' = Rub. Measured $k/(k_d/[A'] + k_A) =$ 2.0×10^{-2} 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 $k_d =$ | Guil.73F333 |
| 4.21 | 2-(2'-hydroxy- 3',5'-di-t-pentyl- phenyl)benzotriazol | i−octane le | < 1 × 10 ⁶ (est) | | rt | A'd-23 | $1.3 \times 10^4 \text{ s}^{-1}$ [1.34]. S = A' = Rub. No measurable effect. | Carl73P066 |
| | C(CH ₂) ₂ CH ₂ | ₂ CH ₃ | | | | | | |
| 4.22 | 2,4,6-triphenyl- phenol | МеОН | 2.52×10^8 | 4.6 × 10 ⁻⁴ | rt | A'd-16 | S = MB, A' = DPF. k derived using $k_d = 1.16 \times 10^5 \text{ s}^{-1}$ ([1.3];[1.3.2];[1.3.3]) ^a . | Thom.78A17 |
| 4.22. | [্] ল'চ 1 | CH₃CN | 1.45×10^7 | 2.3×10^{-3} | rt | A'd-16 | S = MB, A' = DPF. k derived using $k_d = 3.33 \times 10^4$ | Thom.78A17 |
| 4.22. | 2 | C ₆ H ₆ | 2.2×10^7 | 1.87×10^{-3} | rt | A'd-16 | s ⁻¹ [1.17]. S = ZnTPP, A' = DPF. k derived using $k_d = 4.17 \times 10^4$ s ⁻¹ [1.32]. | Thom.78A17 |
| 4.23 | 3,5-di-t-butyl- 4-hydroxyphenyl propionate OCOC ₂ H ₅ (CH ₃ I ₃ C OH | МеОН | 2.18 × 10 ⁵ | 5.34 × 10 ⁻¹ | rt | A'd-16 | | Thom.78A17 |
| 4.24 | durohydro- quinone mono- ethyl ether OH H ₃ C CH ₃ OCH ₂ CH ₃ | МеОН | 7.25×10^{7} | 1.6×10^{-3} | rt | A'd-16 | S = MB, A' = DPF. k derived using $k_a = 1.16 \times 10^5 \text{ s}^{-1}$ ([1.3];[1.3.2];[1.3.3]) ^a . | Thom.78A17 |
| 4.25 | δ-tocopherol CH ₃ CH ₃ CH ₂ C | МеОН Сн ₃ н₂сн 13 сн ₃ | 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 = 8.3×10^4 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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|--|--|--|---------------------------------------|----------|--------------|---|-------------|
| 4.25. | 2 | EtOH | $k_{\rm r}=2.3\times10^6$ | | 20 | P'a-17 Ad | S = MB, A' = methyllinoleate, P' = methyllinoleate hydroperoxide. Measured (k_r^A/k_r) = 9.5×10^{-2} . k_r derived using k_r^A = 2.2×10^5 dm ³ mol ⁻¹ s ⁻¹ [14.6]. | Yama.77F858 |
| 4.26 | β -tocopherol CH ₃ CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃ | MeOH ^{ÇH} ₃ ౫₂сн \ ₃ сн₃ | 3.6×10^8 | $(2.8 \pm 0.2) \times 10^{-4}$ | 25 | Ad-15 | S = MB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | Gram.72A019 |
| 4.27 | γ-tocopherol H ₃ C CH ₃ CH ₂ CH ₂ HO CH ₂ CH ₂ | MeOH CH3 CH2CH3-CH3 | 1.9×10^8 | $(5.4 \pm 0.3) \times 10^{-4}$ | 25 | Ad-15 | S = MB. k derived using $k_d = *1.0 \times 10^5$ 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, $A' = methyl-linoleate, P' = methyl-linoleate hydroperoxide.k derived using k_d = 8.2 \times 10^4 -1 (1)$ | Yama.77F858 |
| 4.27. | 2 | EtOH | $k_{\rm r}=7.9\times10^6$ | | 20 | P'a-17 Ad | 8.3 × 10 ⁴ s ⁻¹ [1.10]. S = MB, A' = methyllinoleate, P' = methyllinoleate hydroperoxide. Measured $(k_r^{A'}/k_r)$ = 2.8 × 10 ⁻² . k_r derived using $k_r^{A'}$ = 2.2 × 10 ⁵ dm ³ mol ⁻¹ s ⁻¹ [14.6]. | Yama.77F858 |
| 4.28 | α -tocopherol H ₃ C CH ₃ CH ₃ (CH ₂ CH | D ₂ O CH ₃ I ₂ CH ₂ CH I ₃ —CH ₃ | 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 | МеОН | 7.1×10^8 | $(1.4 \pm 0.4) \times 10^{-4}$ | 25 | Ad-15 | S = MB. k derived using $k_d = *1.0 \times 10^5$ | Gram.72A019 |
| 4.28. | 2 | МеОН | $(6.7 \pm 0.6) \times 10^{8}$ *4.8 × 10 ⁸ | $(2.1 \pm 0.2) \times 10^{-4}$ | rt | A'd-16 | s ⁻¹ [1.3.6]. S = MB, A' = DPBF. k derived using $k_d = 1.4 \times 10^5$ (*1.0 × 10 ⁵) s ⁻¹ [1.3]. | Foot74R113 |
| 4.28. | 3 | МеОН | $k_{\rm r} = (4.6 \pm 1.0) \times 10^7$ *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 × 10 ⁸ (*7.0 × 10 ⁷) dm ³ mol ⁻¹ | Foot74R113 |
| 4.28. | 4 | CCl₄ | $(1.0 \pm 0.3) \times 10^8$ | | rt | Ld-13 | s^{-1} [A3.16]. $S = ?$ k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ [1.8.3]. | Kras79A010 |

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

| No. Substrate (A) | Solvent | $k / dm^3 \text{ mol}^{-1} \text{ s}^{-1}$ | $\beta (k_d/k)$ /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 = $8.3 \times 10^4 \text{ s}^{-1} [1.10]$. | Yama.77F858 |
| 4.28.6 | EtOH | $k_{\rm r}=2.0\times10^7$ | | 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 $k_r^{A'}$ = 2.2×10^5 dm³ 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 $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc). | Koka.78F404 |
| 4.28.8 | CCl ₂ F- CClF ₂ | $(3.1 \pm 1.2) \times 10^7$ | | rt | A'd-23 | $^{1}O_{2}^{*}$ from Nd-YAG (CW) laser (1065 nm), A' = bilirubin. k derived using $k_{O2} = 2.7 \times 10^{3}$ dm ³ mol ⁻¹ s ⁻¹ (gas phase | Brab.76F425 |
| 4.28.9 | CCl ₂ F- CClF ₂ | $k_{\rm r} = (1.9 \pm 0.5) \times 10^6$ | | rt | Ad-36 | value [74F102]). ${}^{1}O_{2}^{*}$ from Nd-YAG CW laser (1065 nm). k_{1} derived using $k_{02} = 2.7 \times 10^{3}$ dm ³ mol ⁻¹ s ⁻¹ (gas phase value [74F102]). | Brab.76F425 |
| 4.28.10 | C ₅ H ₅ N | $(2.5 \pm 0.1) \times 10^8$ | | rt | A'd-23 | S = A' = Rub. k derived using $k_{A'} = 4 \times 10^7 \text{ dm}^3$ $\text{mol}^{-1} \text{ s}^{-1} [74\text{F2}07]$ and $k_d = *6.0 \times 10^4$ $\text{s}^{-1} [1.29.1]$. | Fahr74R112 |
| 4.28.11 | C ₅ H ₅ N | $k_{\rm r}=1.2\times10^6$ | | rt | Ad-14 28 | | Fahr74R112 |
| 4.28.12 | C ₆ H 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]. | Stev74R114 |
| 4.28.13 | C ₆ H ₁₂ | $k_{\rm r} = 1.1 \times 10^6$ *1.4 × 10 ⁶ | | 25 | Ad-17 A'd | | Stev74R114 |
| 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 β_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]. | Stev74R114 |

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

| No. Substrate (A) | Solvent | /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /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 $k_{A'} = 4 \times 10^7 \text{ dm}^3$ $mol^{-1} \text{ s}^{-1} [74\text{F}207]$ and k_d (unreported). | Fahr74R112 |
| 4.29 α-naphthol | n-BuOH | 3.2×10^7 | | 20 | A'd-23 | S = MB, A' = Tetr. k derived using $k_{A'}$ = $5.2 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.62.3] and k_d = $5.2 \times 10^4 \text{ s}^{-1}$ [1.24]. | Snya78A266 |
| 4.30 β-naphthol | n-BuOH | $7.6 	imes 10^6$ | | 20 | A'd-23 | S = MB, A' = Tetr. k derived using $k_{A'}$ = 5.2×10^8 dm ³ mol ⁻¹ s ⁻¹ $[3.62.3]$ and k_d = 5.2×10^4 s ⁻¹ $[1.24]$. | Snya78A266 |
| 4.31 hydroquinone | C ₅ H ₅ N | 6.9×10^{7} | | rt | A'd-23 | S = A' = Rub. k derived using $k_{A'}$ = $4 \times 10^7 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [74F207] and $k_d = *6.0 \times 10^4$ s ⁻¹ [1.29.1]. | Fahr74R112 |
| 4.31.1 | C ₆ H ₆ /MeOH (4:1) v:v | 7.0×10^{7} *2.7 × 10 ⁷ | • | 25 | P'a-20 | S = MB, A' = 2M2P. k derived using $\beta_{A'} = 4 \times 10^{-2} \text{ mol}$ dm^{-3} and $k_d = 1.0 \times 10^5$ (*3.8 × 10 ⁴) s ⁻¹ [1.49]. | Foot70F734 |
| 4.31.2 | EtOH/H ₂ (95:5) v:v | $O(5.8 \pm 2.4) \times 10^8$ | | rt | Ld-13 | O 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-tetra- methylbutyl)phen | i-octane | $< 1.0 \times 10^6$ (est) | | rt | A'd-23 | S = A' = Rub. No measurable effect. | Carl73P066 |
| (CH ₃) ₃ C CH ₂ C(CH ₃) ₂ | OH C(CH3)2CH2C(CH3)3 | | | | | | |
| 4.33 (CH ₃) ₃ C OH CH ₂ | CH ₂ Cl ₂ | 8.2 × 10 ⁹ | | 30 | Od-23 | S = MB, A' = TME. k derived using $k_{A'}$ = *3.0 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [A3.2] and k_d = *1.2 × 10 ⁴ s ⁻¹ [I.4.2]. | Taim.76F921 |

 $^{{}^{\}mathrm{a}}$ 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

| o. Substrate (A) | Solvent | $\frac{k}{\text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | <i>t</i> /°℃ | Method | Comments | Ref. |
|------------------|-------------|---|---|-----------------|--------|----------|------|
| | Notes & ren | recents the everell re | to constant unless k (c) | homical read | | | |

or $k_{\rm q}$ (quenching rate constant) is specified; $k_{\rm d}$ is the rate constant for solvent deactivation]

COMPOUNDS 5.1 - 5.33:

| | | | | 5 2 | | | | |
|--------|-----------------------------|------------------------------|-----------------------|--------------------------------|----|--------|---|-------------|
| 5.1 | furan | МеОН | 2.2×10^{7} | 4.5×10^{-3} | 20 | Od-15 | using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a =$ | Koch68F288 |
| 5.1.1 | | МеОН | 3.8×10^7 | 2.6×10^{-3} | rt | A'd-16 | 0.84 kJ mol ⁻¹ . S = MB, A' = DPBF. k derived using $k_a = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | Youn72F510 |
| 5.2 | 2-methylfuran $[R_2 = -Me]$ | H ₂ O (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 ₂ O (pH 7.0) | 1.1×10^{8} | | rt | Od-19 | S = chlorophyll-a, Q = N ₃ ⁻ . k derived using $k_Q = 2 \times 10^8$ dm³ mol ⁻¹ s ⁻¹ [12.9.6]. S solubilized in Triton X-100 micelles (2% by volume). | Barb.78A278 |
| 5.2.2 | | H ₂ O (pH 7.0) | 1.0×10^8 | | rt | Od-19 | S = chlorophyll-a, $Q = N_3^- k$ derived using $k_Q = 2 \times 10^8$ dm³ mol ⁻¹ s ⁻¹ [12.9.6]. S solubilized in Triton X-100 micelles (5% by volume). | Barb.78A278 |
| 5.2.3 | | H ₂ O (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 ₂ O (pH 7.0) | 6.0×10^{7} | • | rt | Od-19 | | Barb.78A278 |
| .5.2.5 | | МеОН | 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 | | МеОН | 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]. | Youn71F398 |
| 5.2.7 | | МеОН | 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]. | Youn72F510 |
| | | | | | | | o [1.J.V]. | |

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

| No. | Substrate (A) | Solvent /c | $\frac{k}{\text{lm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $(\beta = k_{\rm d}/k)$ /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 $k_d = 5.2 \times 10^4 \text{ s}^{-1}$ [1.24]. | Youn71F398 |
| 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 $k_d = 3.0 \times 10^4 \text{ s}^{-1}$ [1.25]. | Youn71F398 |
| 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 | | МеОН | 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]. | Youn72F51 |
| 5.4 | furfural [R ₂ = -CHO] | МеОН | 1.7 × 10 ⁵ | 6.0×10^{-1} | 20 | Od-15 | S = RB. k derived using $k_d = *1.0 \times 10^5$ $s^1 [1.3.6]. E_a = 21 \text{ kJ mol}^{-1}$. | Koch68F288 |
| 5.4.1 | 5 | МеОН | 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]. | Youn72F51 |
| 5.5 | 2-methoxyfuran $[R_2 = -OMe]$ | МеОН | 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]. | Youn72F51 |
| 5.6 | furfuryl alcohol $[R_2 = -CH_2OH]$ | H_2O | 2.4×10^8 | 1.8×10^{-3} | rt | Od-14 | | Sluy61F008 |
| 5.6,1 | | МеОН | 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 | | МеОН | 2.1×10^{7} | 4.7×10^{-3} | rţ | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. | Youn72F51 |
| 5.7 | furfuryl- methylether | МеОН | 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] | МеОН | 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]. | Youn72F51 |
| 5.9 | 2-vinylfuran [R2 = -CH=CH2] | МеОН | 5.6×10^7 | 1.8×10^{-3} | 20 | Od-15 | S = RB. k derived using $k_d = *1.0 \times 10^5$ $s^{-1} [I.3.6]. E_a = 3.8 \text{ kJ mol}^{-1}$. | Koch68F288 |
| 5.10 | α -methylfurfuryl alcohol [R ₂ = -CH(OH)C | MeOH | 1.04 × 10 ⁸ | 8.73×10^{-4} | 25 | A'd-16 | S = RB, A' = DPBF. k derived using k_d = $9.0 \times 10^4 \text{ s}^{-1}$ ([1.3.2];[1.3.3]). ^b | Mart72F519 |
| 5.11 | α -phenylfurfuryl alcohol [$R_2 = -CH(OH)C$ | MeOH | 5.15 × 10 ⁶ | 1.77×10^{-2} | 25 | · A'd-16 | S = RB, A' = DPBF. k derived using k_d = $9.0 \times 10^4 \text{ s}^{-1}$ ([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. S | Substrate (A) | Solvent /d | $\frac{k}{\text{lm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|---|---|---|----------|-----------------------|--|------------|
| 5.12 | α -benzylfurfuryl alcohol [R ₂ = -CH(OH)CH | MeOH | 1.09 × 10 ⁷ | 8.35 × 10 ⁻³ | 25 | A'd-16 | S = RB, A' = DPBF. k derived using k_d = $9.0 \times 10^4 \text{ s}^{-1}$ | Mart72F519 |
| 5.13 | α -phenethyl- furfuryl alcohol [$R_2 = -CH(OH)(C$ | MeOH H ₂) ₂ C ₆ H ₅] | 2.54×10^7 | 3.58×10^{-3} | 25 | A'd-16 | ([1.3.2];[1.3.3]. ^b S = RB, A' = DPBF. k derived using k_d = $9.0 \times 10^4 \text{ s}^{-1}$ ([1.3.2];[1.3.3]. ^b | Mart72F519 |
| 5.14 | α -(3-phenylpropyl) furfuryl alcohol [$R_2 = - CH(OH)(C)$ | • | 8.94×10^{8} | 1.02 × 10 ⁻⁴ | 25 | A'd-16 | S = RB, A' = DPBF. k derived using k_d = $9.0 \times 10^4 \text{ s}^{-1}$ | Mart72F519 |
| 5.15 | α -benzhydryl- furfuryl alcohol $[R_2 = -CH(OH)CH]$ | MeOH H(C ₆ H ₅) ₂] | 1.14×10^7 | 8.0×10^{-3} | 25 | A'd-16 | $([1.3.2];[1.3.3])^b$ S = RB, A' = DPBF. k derived using k_d = $9.0 \times 10^4 \text{ s}^{-1}$ | Mart72F519 |
| 5.16 | α , α -diphenylfur- furyl alcohol [$R_2 = -C(OH)(C_6H)$] | MeOH I₅) ₂] | 9.9 × 10 ⁶ | 9.2×10^{-3} | 25 | A'd-16 | ([1.3.2];[1.3.3]. ^b S = RB, A' = DPBF. k derived using k_d = $9.0 \times 10^4 \text{ s}^{-1}$ | Mart72F519 |
| 5.17 | 2-acetylfuran [R ₂ = -COCH ₃] | МеОН | 4.5×10^6 | 2.2×10^{-2} | rt | A'd-16 | ([1.3.2];[1.3.3]. ^b S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ | Youn72F5 |
| 5.18 | N-methylfurfuryl- amine $[R_2 = -CH_2NH(CH_2)]$ | | 7.7×10^6 | 1.3×10^{-2} | 20 | Od-15 | s^{-1} [1.3.6]. $S = RB$. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. $E_a =$ 4.2 kJ mol ⁻¹ . | Koch68F288 |
| 5.19 | 2-phenylfuran [R ₂ = -Ph] | МеОН | $k_{\rm r}=3.9\times10^7$ | | 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]. | Youn71F398 |
| 5.19.1 | | МеОН | $k_{\rm r}=3.9\times10^7$ | | rt | Ad-17 A'd | | .Youn72F5 |
| 5.19.2 | | n-BuOH | $k_{\rm r} = 2.6 \times 10^7$ *1.8 × 10 ⁷ | $ \beta_{\rm r} = 2.0 \times 10^{-3} \\ *2.9 \times 10^{-3} $ | 25 | Ad-17 A'd (sep) | | Youn71F398 |
| 5.19.3 | | t-BuOH | $k_{\rm r} = 8.8 \times 10^6$ *6.0 × 10 ⁶ | $ \beta_{\rm r} = 3.4 \times 10^{-3} \\ *5.0 \times 10^{-3} $ | 25 | Ad-17 A'd (sep) | | Youn71F398 |
| 5.20 | 3 -phenylfuran [$R_3 = -Ph$] | МеОН | 3.6×10^7 | 2.8×10^{-3} | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | Youn72F5 |
| 5.21 | $3-(4'-fluoro-phenyl)furan$ [$R_3 = 4'-FC_6H_4-$] | МеОН | 2.9×10^7 | 3.4×10^{-3} | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. | Youn72F5 |

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

| No. | Substrate (A) | Solvent /c | $\lim_{n \to \infty} \frac{k}{m o l^{-1}} s^{-1}$ | $(\beta = k_{d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments Ref. | |
|--------|--|---------------------------------------|---|--|----------|-----------------------|---|-----------------|
| 5.22 | 2-(4'-chloro- phenyl)furan $[R_2 = 4'-ClC_6H_4-$ | МеОН | $k_{\rm r}=2.5\times10^7$ | | 25 | Ad-17 A'd | S = RB, A' = DPF. Youn Measured $(k_r/k_r^{A'})$ = 0.352. k_r derived using $k_r^{A'}$ = *7.0 × 10 ⁷ | 71F398 |
| 5.22.1 | | МеОН | 3.4×10^{7} | 2.9×10^{-3} | rt | A'd-16 | dm ³ mol ⁻¹ s ⁻¹ [A3.16]. S = MB, A' = DPBF. Youn k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | 72F51 |
| 5.22.2 | | n-BuOH | $k_{\rm r} = 1.5 \times 10^7$ *1.0 × 10 ⁷ | $ \beta_{\rm r} = 3.4 \times 10^{-3} $ *5.0 × 10 ⁻³ | . 25 | Ad-17 A'd (sep) | S = RB, A' = DPF. Youn Measured (β_r/β_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 $k_d = 5.2 \times 10^4$ s ⁻¹ [1.24]. | 71F398 |
| 5.22.3 | | t-BuOH | $k_{\rm r} = 8.6 \times 10^5$ *5.8 × 10 ⁵ | $ \beta_{\rm r} = 3.5 \times 10^{-2} \\ *5.2 \times 10^{-2} $ | 25 | Ad-17 A'd (sep) | 5.2×10^{-8} (MeOH)) = 36.8. 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 [1.24]. | 71 F 398 |
| 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. Youn k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | 72F51 |
| 5.24 | $2-(4'-methyl-phenyl)$ furan [$R_2 = 4'-CH_3C_6H_1$] | MeOH ₄~] | $k_{\rm r}=4.8\times10^7$ | | rt | Ad-17 A'd | S=MB or RB, A' = DPF. Youn 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]. | 72F51 |
| 5.25 | $3-(4'-methyl-phenyl)$ furan [$R_3 = 4'-CH_3C_6H_3$] | MeOH ₄~] | 4.2×10^7 | 2.4×10^{-3} | rt | A'd-16 | S=RB or MB, A' = DPBF. Youn k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. | 72F51 |
| 5.26 | 2- $(4'$ -methoxy-phenyl)furan [R ₂ = $4'$ -MeOC ₆ F | H ₂ O I ₄ –] | $k_{\rm r} = 7.5 \times 10^8$ *5.1 × 10 ⁸ | $ \beta_{\rm r} = 5.9 \times 10^{-4} \\ *8.7 \times 10^{-4} $ | rt | Ad-17 A'd (sep) | S=MB or RB, A' = DPF. Youn Measured $(\beta_r/\beta_r^{A'}(MeOH))$ = 0.618. k_r derived using $\beta_r^{A'} = 9.5 \times 10^{-4}$ (*1.4 × 10 ⁻³) mol dm ⁻³ [5.30.5] and $k_d =$ *4.4 × 10 ⁵ s ⁻¹ [1.1.3]. | 72 F 51 |
| 5.26.1 | | МеОН | $k_{\rm r}=6.4\times10^7$ | | rt | Ad-17 A'd | S=MB or RB, A' = DPF. Youn 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]. | 72F510 |
| 5.26.2 | | glycol | $k_{\rm r} = 4.7 \times 10^8$ *3.2 × 10 ⁸ | $ \beta_{\rm r} = 3.4 \times 10^{-4} \\ *5.0 \times 10^{-4} $ | rt | Ad-17 A'd (sep) | S=MB or RB, A' = DPF. Youn Measured $(\beta_r/\beta_r^{A'}(MeOH))$ = 0.36. k_r derived using $\beta_r^{A'} = 9.5 \times 10^{-4}$ (*1.4 × 10 ⁻³) mol dm ⁻³ [5.30.5] and $k_d =$ *1.6 × 10 ⁵ s ⁻¹ [1.11.1]. | 72F510 |
| 5.26.3 | | n-BuOH | $k_{\rm r} = 2.7 \times 10^7$ *1.9 × 10 ⁷ | $ \beta_{\rm r} = 1.9 \times 10^{-3} \\ *2.8 \times 10^{-3} $ | rt | Ad-17 A'd (sep) | | 72F51 |

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

| No. S | ubstrate (A) | Solvent / | k 'dm³ mol ⁻¹ s ⁻¹ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|--|------------------|---|---|----------|--------|---|-------------|
| 5.27 | 3-(4'-methoxy- phenyl)furan [R ₃ = 4'-MeOC ₆ H | MeOH | 5.3 × 10 ⁷ | 1.9 × 10 ⁻³ | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ | Youn72F510 |
| 5.28 | 2,4-dimethylfuran $[R_2 = R_4 = -Me]$ | МеОН | 5.0 × 10 ⁷ | 2.0×10^{-3} | 20 | Od-15 | s ⁻¹ [1.3.6]. 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 $[R_2 = R_5 = -Me]$ | | 1.7×10^9 *1.5 × 10° | $(3.0 \pm 0.6) \times 10^{-4}$ | 25 | Ad-15 | S = MB. k derived using $k_d = 5.0 \times 10^5$ (*4.4 × 10 ⁵) s ⁻¹ [1.1]. | Usui.74F044 |
| 5.29.1 | | H ₂ O | 1.56×10^9 | 3.2×10^{-4} | 25 | Ad-15 | | Usui78F061 |
| 5.29.2 | | H ₂ O | 1.5×10^9 *1.4 × 10° | $(3.2 \pm 0.6) \times 10^{-4}$ | 25 | Ad-15 | | Usui.74F044 |
| i.29.2a | ı | H ₂ O | 8.0×10^8 | 5.5×10^{-4} | 25 | Od-15 | $^{1}O_{2}^{*}$ from $H_{2}O_{2}/NaOCl$. k derived using $k_{d} = *4.4 \times 10^{5} \text{ s}^{-1}$ [1.1.3]. | Held78A227 |
| 5.29.3 | | МеОН | $\sim 5.0 \times 10^8$ | $\sim 2.0 \times 10^{-4}$ | 20 | Od-15 | | Koch68F288 |
| 5.29.4 | | МеОН | 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]. | Youn71F398 |
| .29.5 | | MeOH | $(4.0 \pm 1.0) \times 10^8$ | | rt | A'd-5 | S = MB, A' = DPBF, | Merk.72F260 |
| .29.6 | | МеОН | 3.6×10^8 | 2.8×10^{-4} | rt | A'd-16 | ruby laser (694 nm). S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. | Youn72F51 |
| .29.7 | e e | МеОН | 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 |
| .29.8 | | МеОН | 3.9×10^8 | 2.8×10^{-4} | 25 | Ad-15 | | Usui78F061 |
| .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]. | |
| 5.29.10 |) | EtOH | 3.8×10^8 | 2.2×10^{-4} | 25 | Ad-15 | | Usui78F061 |
| 5.29.11 | | EtOH | 4.9×10^8 | 1.6 × 10 ⁻⁴ | rt | Ad-15 | | Delm.78F201 |
| 5.29.12 | 2 | 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 /dm³ mol ⁻¹ s ⁻¹ | $(\beta = k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---|---|--|----------|-----------------------|---|-------------|
| 5.29.13 | $CFCl_2$ - 8.0×10^6 CF_2Cl (est) | | rt | A'd-37 | $^{1}O_{2}$ * from Nd-YAG CW laser (1065 nm), A' = Rub. Measured $k/k_{O2}[O_{2}] = 2 \times 10^{3}$ dm ³ mol ⁻¹ . k estimated using $k_{O2}[O_{2}] = 4 \times 10^{3}$ s ⁻¹ (based on gas phase value of $k_{O2} = 1.3 \times 10^{3}$ dm ³ mol ⁻¹ s ⁻¹). | Math.70F387 |
| 5.29.14 | $(Me)_2CO$ 2.1 × 10 ⁸ $+1.7 \times 10^8$ | 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 $k_{\rm r} = 7.2 \times 10^7$ /t-BuOH (1:1) v:v | | 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 [43.2]. | Higg68F292 |
| 5.29.16 | MeOH $k_{\rm r} = 1.6 \times 10^8$ /t-BuOH (1:1) v:v | | rt | Ad-17 A'd | $^{1}O_{2}*$ from $H_{2}O_{2}/NaOCl$, A' = TME. Measured $(k_{r}/k_{r}^{A'}) = 5.2$. k_{r} derived using $k_{r}^{A'} =$ $^{*}3.0 \times 10^{7}$ dm ³ $^{*}mol^{-1}$ s ⁻¹ [43.2]. | Higg68F292 |
| 5.29.17 | MeOH $k_{\rm r} = $ /t-BuOH 4.5 × 10 ⁷ (1:1) v:v | | rt | Ad-17 A'd | $^{1}O_{2}$ * from $H_{2}O_{2}/Ca(OCl)_{2}$, $A' = TME$. Measured $(k_{r}/k_{r}^{A'}) = 1.5$. k_{r} derived using $k_{r}^{A'} = *3.0 \times 10^{7} \text{ dm}^{3}$ mol ⁻¹ s ⁻¹ [43.2]. | Higg68F292 |
| 5.29.18 | MeOH 4.9 × 10 ⁸ /t-BuOH (est) (1:1) v:v For more relative rates see | $(1.6 \pm 0.2) \times 10^{-4}$ | rt | A'd-16 | S = RB, A' = DPBF. k estimated using k_d = $7.9 \times 10^4 \text{ s}^{-1}$ (cale). | Youn71F398 |
| 5.30 2,5-diphenylfuran $[\mathbf{R}_2 = \mathbf{R}_5 = -\mathbf{Ph}]$ | _ | 7.17, 7.17.1. $\beta_r =$ 4.58 × 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) and dm^{-3} [5.30.5] and $k_d =$ | Youn71F398 |
| 5.30.1 | D_2O $k_r = 4.0 \times 10^8$ | $\beta_{\rm r} = 7.7 \times 10^{-5}$ | 23 | Ad-17 A'd (sep) | *4.4 \times 10 ⁵ s ⁻¹ [<i>I.1.3</i>]. 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 \times 10 ⁴ s ⁻¹ [1.2.3]. | Port.74R214 |
| 5.30.2 | D_2O $k_r = 2.5 \times 10^8$ (pD 7.1) | $\beta_{\rm r} = 1.2 \times 10^{-4}$ | 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 $k_d = *3.1 \times 10^4$ s ⁻¹ [1.2.3]. | Port.74R214 |
| 5.3 ò .3 | D_2O $k_r = 2.2 \times 10^8$ (pD 7.1) | $\beta_{\rm r} = 1.4 \times 10^{-4}$ | 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 $k_d = *3.1 \times 10^4 \text{ s}^{-1}$ [1.2.3]. solvent contains 960 μ M H ₂ O 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 /c | $\lim_{n \to \infty} \frac{k}{n}$ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|---------------------------------|--|---|----------|-----------------------|--|-------------|
| 5.30.4 | D ₂ O (pD 7.1) | $k_{\rm r}=2.8\times10^8$ | $\beta_r = 1.1 \times 10^{-4}$ | 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 $k_d = *3.1 \times 10^4$ s ⁻¹ [1.2.3]. 1 μ 1/ml of catalase present in reaction medium. | Port.74R214 |
| 5.30.5 | МеОН | 1.1×10^{8} | $(9.5 \pm 1.0) \times 10^{-4}$ | 25 | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. | Youn71F39 |
| 5.30.6 | МеОН | $(4.6 \pm 0.8) \times 10^7$ | | rt | A'd-8 | S = RB, A' = DPBF, dye laser (583 nm). ^a | Youn73F01 |
| 5.30.7 | МеОН | $k_{\rm r} \approx 5 \times 10^5$ $*3.6 \times 10^5$ | | 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 | МеОН | 1.1 × 10 ⁸ | 8.82×10^{-4} | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ s ¹ [1.3.6]. | Brew74F646 |
| 5.30.9 | CH ₂ Cl ₂ | 8.6×10^7 | 1.39 × 10 ⁻⁴ | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *1.2 \times 10^4$ 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 $k_d = *1.0 \times 10^4$ s^{-1} [1.5.3]. | Brew74F646 |
| 5.30.11 | glycol | $k_{\rm r} = 4.6 \times 10^8$ *3.1 × 10 ⁸ | $ \beta_{\rm r} = 3.5 \times 10^{-4} \\ *5.1 \times 10^{-4} $ | rt | Ad-17 A'd (sep) | S = RB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.366$. k_r derived using $\beta_r(\text{MeOH}) = 9.5 \times 10^{-4}$ (*1.4 × 10 ⁻³) mol dm ⁻³ [5.30.5] and $k_d = 1.6 \times 10^5 \text{ s}^{-1}$ [1.11.1]. | Youn71F39 |
| 5.30.12 | CH ₃ CN | 2.0×10^{8} | 1.3×10^{-4} | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *2.55 \times 10^4$ s ⁻¹ [1.17.2]. | Brew74F646 |
| 5.30.13 | <i>i</i> -PrOH | 4.8×10^{7} | 1.04×10^{-3} | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = 5.0 \times 10^4 \text{ s}^{-1}$ [1.19]. Solvent contained 1% MeOH. | Brew74F646 |
| 5.30.14 | (Me) ₂ CO | 1.8 × 10 ⁸ | 1.7 × 10 ⁻⁴ | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *3.1 \times 10^4$ s^{-1} [1.22.2]. | Brew74F646 |
| 5.30.15 | n-BuOH | $k_{\rm r} = 5.3 \times 10^7$ *3.6 × 10 ⁷ | $ \beta_{\rm r} = 9.8 \times 10^{-4} \\ *1.4 \times 10^{-3} $ | 25 | Ad-17 A'd (sep) | S = RB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 1.03$. k_r derived using $\beta_r(\text{MeOH}) = 9.5 \times 10^{-4}$ (*1.4 × 10 ⁻³) mol dm ⁻³ [5.30.5] and $k_d = 5.2 \times 10^4 \text{ s}^{-1}$ [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 /c | $\frac{k}{\text{lm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $(\beta \approx k_{\rm d}/k)$ /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 $k_d = 5.2 \times 10^4 \text{ s}^{-1}$ [1.24]. Solvent contained 1% MeOH. | Brew74F646 |
| 5.30.17 | t-BuOH | $k_{\rm r} = 3.75 \times 10^7$ *2.5 × 10 ⁷ | $ \beta_{\rm r} = 8.0 \times 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 $k_d = 3.0 \times 10^4 \text{ s}^{-1}$ [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 $k_d = 3.0 \times 10^4 \text{ s}^{-1}$ [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 $k_d = 2.1 \times 10^4 \text{ s}^{-1}$ [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 $k_d = 2.9 \times 10^4 \text{ s}^{-1}$ [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 $k_d = 4.3 \times 10^4 \text{ s}^{-1}$ [1.26]. | Brew74F646 |
| 5.30.22 | C₅H₅N | 6.1×10^7 | 9.9 × 10 ⁻⁴ | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *6.0 \times 10^4 \text{ s}^{-1}$ [1.29.1]. Solvent contained 1% MeOH. | Brew74F646 |
| 5.30.23 | C ₆ H ₁₁ OH | 5.3×10^7 | 1.17×10^{-3} | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = 6.2 \times 10^4 \text{ s}^{-1}$ [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 $k_d = 2.5 \times 10^4 \text{ s}^{-1}$ [1.37]. Solvent contained 1% MeOH. | Brew74F646 |
| 5.30.25 | MeOH/H ₂ (81:19) Mole % | $_{2}0 k_{r} = 2.9 \times 10^{8}$ $_{1.9} \times 10^{8}$ (est) | $ \beta_{\rm r} = $ $ 7.7 \times 10^{-4} $ *1.1 × 10 ⁻³ | rt | Ad-17 A'd (sep) | | Youn71F398 |
| 5.30.26 | MeOH/H (66:34) Mole % | $_{2}0 k_{r} = 4.7 \times 10^{8}$ $_{3.2} \times 10^{8}$ (est) | $ \beta_{\rm r} = 5.9 \times 10^{-4} \\ *8.7 \times 10^{-4} $ | rt | Ad-17 A'd (sep) | S = RB. Measured $(\beta_r/\beta_r(MeOH)) = 0.621$. k_r estimated using $\beta_r(MeOH) = 9.5 \times 10^{-4}$ $(*1.4 \times 10^{-3})$ mol dm ⁻³ $[5.30.5]$ and $k_d = 2.8 \times 10^5$ s ⁻¹ (calc). | Youn71F398 |

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

| No. Subs | trate (A) | Solvent /d | $\frac{k}{\text{lm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $(\beta = k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|----------|---|--|--|---|------------------------------|------------------------------|--|--------------|
| 5.30.27 | | MeOH/H (40:60) Mole % | $_{2}0 k_{r} = 8.5 \times 10^{8}$ $*5.8 \times 10^{8}$ (est) | $ \beta_{\rm r} = 4.2 \times 10^{-4} \\ *6.2 \times 10^{-4} $ | rt | Ad-17 A'd (sep) | S = RB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.446$. 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 = | Youn71F398 |
| 5.30.28 | | MeOH/H (12:88) Mole % | $k_2 0 k_r = 1.0 \times 10^9$ *6.8 × 10 ⁸ (est) | $ \beta_{\rm r} = 4.2 \times 10^{-4} \\ *6.1 \times 10^{-4} $ | rt | Ad-17 A'd (sep) | 3.6 × 10 ⁵ s ⁻¹ (calc). S = RB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.439$. k_r estimated using $\beta_r(\text{MeOH}) = 9.5 \times 10^{-4}$ (*1.4 × 10 ⁻³) mol dm ⁻³ [5.30.5] and $k_d = 4.2 \times 10^5$ s ⁻¹ (calc). | Youn71F398 |
| 5.30.29 | | MeOH /glycol (3:1) v:v | 2.0×10^{8} *1.4 × 10 ⁸ (est) | $ \beta_{\rm r} = 5.5 \times 10^{-4} \\ *8.1 \times 10^{-4} $ | rt | Ad-17 A'd (sep) | $S = RB$. Measured $(\beta_r/\beta_r(MeOH)) = 0.578$. k_r derived using $\beta_r(MeOH) = 9.5 \times 10^{-4}$ (*1.4 × 10 ⁻³) mol dm ⁻³ [5.30.5] and $k_d = 1.1 \times 10^5 \text{ s}^{-1}$ (calc). | Youn71F398 |
| 5.30.30 | | MeOH /glycol (1:1) v:v | 3.8×10^{8} *2.6 × 10 ⁸ (est) | $ \beta_{\rm r} = 3.4 \times 10^{-4} \\ *5.0 \times 10^{-4} $ | rt | Ad-17 A'd (sep) | S = RB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.355$. k_r derived using $\beta_r(\text{MeOH}) = 9.5 \times 10^{-4}$ (*1.4 × 10 ⁻³) mol dm ⁻³ [5.30.5] and $k_d = 1.3 \times 10^5 \text{ s}^{-1}$ (calc.). | Youn.,71F398 |
| 5.30.31 | | MeOH /glycol (1:3) v:v | 5.4×10^{8} *3.6 × 10 ⁸ (est) | $ \beta_{\rm r} = 2.6 \times 10^{-4} \\ *3.9 \times 10^{-4} $ | rt . | Ad-17 A'd (sep) | 1.3 \times 10.5 (calc.). S = RB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.278$. k_r derived using $\beta_r(\text{MeOH}) = 9.5 \times 10^{-4}$ $(*1.4 \times 10^{-3})$ mol dm ⁻³ [5.30.5] and $k_d = 1.4 \times 10^5$ s ⁻¹ (calc). | Youn71F398 |
| | | For more | relative rates see | 4.28.3, 5.19, 5.19. 5.26.1–3, 5.36.7, 5.36.55, 5.36.58, 5.36.74, 5.36.78, 5 | .36.13, 5.36 .36.61, 5.36 | 5.21, 5.36.2 5.64–5, 5.36 | 24, 5.26, 5, 5.36.42, 5.36.45, | |
| | A-diphenylfuran $A_3 = R_4 = -Ph$ | МеОН | 6.0×10^7 | 1.67×10^{-3} | rt | | S=RB or MB, A' = DPB k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | F. Youn72F51 |
| ca | 4-diethoxy- arbonylfuran $R_3 = R_4 = -CO$ | MeOH OC ₂ H ₅] | $\approx 5.0 \times 10^5$ | $\approx 2.0 \times 10^{-1}$ | 20 | Od-15 | S = RB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a =$ 12.6 kJ mol ⁻¹ . | Koch68F288 |
| ph | 3,4,5-tetra- nenylfuran $R_2 = R_3 = R_4 = R_4$ | МеОН | $\approx 3.3 \times 10^6$ | $\approx 3.0 \times 10^{-2}$ | 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 |
| | R ₅ = -Ph] 2(2,5)furan- phane | МеОН | 1.6×10^8 | 5.47 × 10 ⁻⁴ | 25 | A'd-16 | 4.2 kJ mol ⁻ . S = RB, A' = DPBF. k derived using $k_d = 9.0 \times 10^4 \text{ s}^{-1}$ $([1.3.2], [1.3.3]).^b$ | Mart72F519 |

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

| No. S | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|------------------|--|---|-----------|--------------|--|-------------|
| | | | | COMPOUNDS 5.3 | 35 – 5.39 | : | | |
| | | | | 5 0 3 | 0 | • | | |
| 5.35 | isobenzofuran | МеОН | 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 | Youn.72F517 |
| .36 | 1,3-diphenyliso- benzofuran $[R_1 = R_3 = -Ph]$ | H ₂ O | 4.5 × 10 ⁹ | $(9.7 \pm 0.8) \times 10^{-5}$ | rt | Ad-15 | $k_{\rm d} = *4.4 \times 10^5 \rm s^{-1}$ [1.1.3]. A solubilized | Gorm76F24 |
| 5.36.1 | | H_2O | 2.2×10^{10} | | 40 | Ad-23 | in SDS micelles. $S = Py$, $A' = NaN_3$. k derived using $k_d = 5.0 \times 10^5 \text{ s}^{-1} [I.I]$. S and A' solubilized in SDS micelles. | Miyo.78A174 |
| 5.36.2 | | H ₂ O | 2.8 × 10 ¹⁰ | | 40 | Ad-23 | | Miyo.78A174 |
| .36.3 | | H_2O | 4.71 × 10° | 1.1 × 10 ⁻⁴ | 25 | Ad-15 | S = MB. k derived using $k_d = 5.0 \times 10^5 \text{ s}^{-1}$ [1.1]. S and A solubilized in SDS micelles. | Usui78F061 |
| .36.4 | | H ₂ O | 4.2 × 10 ⁹ | 1.2×10^{-4} | 25 | Ad-15 | S = Eos. k derived using $k_d = 5.0 \times 10^5 \text{ s}^{-1}$ [$l.1$]. A solubilized in SDS micelles. | Usui78F061 |
| .36.5 | | D ₂ O | 8.4×10^8 | | rt | Ad-5 | $S=2$ -acetonaphthone, N_2 laser (337 nm). S and A solubilized in SDS micelles. | Gorm.78E14 |
| .36.6 | | МеОН | $\approx 7.7 \times 10^6$ | $\approx 1.3 \times 10^{-2}$ | 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 |
| .36.7 | | МеОН | $k_{\rm r}=9.1\times10^8$ | | 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 [<i>A3.16</i>]. | Youn71F398 |
| .36.8 | | MeOH | $(7.0 \pm 1.0) \times 10^8$ | | rt | Ad-5 | S = MB, ruby laser (694 nm). | Merk.71M325 |
| .36.9 | | MeOH | $(8.0 \pm 2.0) \times 10^8$ | | rt | Ad-5 | S = MB, ruby laser (694 nm). | Merk.72F260 |
| .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 | Youn73F014 |
| 36.11 | | MeOH | $(1.2 \pm 0.4) \times 10^9$ | $(8.1 \pm 1.5) \times 10^{-5}$ | rt | A d-8 | S = RB, dye laser (583 nm). ^a | Youn73F014 |
| .36.12 | | МеОН | $k_{\rm r} = 6.13 \times 10^8$ *4.38 × 10 ⁸ | $\beta_{\rm r} = 2.27 \times 10^{-4}$ | rt | Ad-14 | S = RB. k derived using $k_d = 1.4 \times 10^5$ (*1.0 × 10 ⁵) s ⁻¹ [1.3] and $\phi_{\rm isc} = 0.76$. | 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 /dm³ mol ⁻¹ s ⁻¹ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | <i>t</i> /°C | Method | Comments | Ref. |
|-------------------|---------------------------------|--|---|-----------------|-----------------------|---|------------------------------|
| 5.36.13 | МеОН | $k_{\rm r} = 1.4 \times 10^9$ *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 × 10 ⁸ (*7.0 × 10 ⁷) dm ³ mol ⁻¹ | Brew74F646 |
| 5.36.14 | МеОН | 1.4×10^9 | $(7.0 \pm 2.6) \times 10^{-5}$ | rt | Ad-15 | s ⁻¹ [A3.16]. S = MB. k derived using $k_d = *1.0 \times 10^5$ | Brew74F646 |
| 5.36.15 | МеОН | 1.6×10^{9} | $(6.4 \pm 0.8) \times 10^{-5}$ | rt | Ad-15 | using $k_{\rm d} = *1.0 \times 10^5$ | Gorm76F24 |
| 5.36.16 | МеОН | $(1.0 \pm 0.1) \times 10^9$ | 1.1×10^{-4} | 20 | Ad-14 | s ⁻¹ [1.3.6]. S = acridine orange. k derived using $k_d = 1.1 \times 10^5 \text{ s}^{-1}$ [1.3.5]. Complicated kinetic treatment. | Schm.76F105 |
| 5.36.17 | МеОН | 7.8×10^8 *5.6 × 10 ⁸ | | rt | Ad-23 | | M iyo.78 A 174 |
| 5.36.18 | МеОН | 1.62 × 10° | 6.8×10^{-5} | 25 | Ad-15 | S = MB. k derived using $k_d = 1.1 \times 10^5$ s^{-1} [1.3.5]. | Usui78F061 |
| 5.36.19 | МеОН | 1.64×10^{9} | | 25 | Ad-5 | S = MB, ruby laser | Usui78F061 |
| 5.36.20 | МеОН | 1.55×10^{9} | 7.1×10^{-5} | 25 | Ad-15 | (694 nm). S = Ery. k derived using $k_d = 1.1 \times 10^5$ | Usui78F061 |
| 5.36.21 | CH ₂ Cl ₂ | $k_{\rm r} = 6.3 \times 10^8$ *5.1 × 10 ⁸ | | rt | Ad-17 A'd (sep) | s ⁻¹ [1.3.5]. S = MB, A' = DPF. Measured $(k_r/k_r^{A'})$ = 7.3. k_r derived using $k_r^{A'}$ = 8.6 × 10 ⁷ (*7.0 × 10 ⁷) dm ³ mol ⁻¹ | Brew74F646 |
| 5.36.22 | CH ₂ Cl ₂ | $(8.2 \pm 2.0) \times 10^8$ | | rt | A d-8 | s^{-1} [A3.16]. S = MB, dye laser | Brew74F646 |
| 5.36.23 | CH ₂ Cl ₂ | 1.08×10^9 | | 25 | Ad-5 | (610 nm). ^a S = MB, ruby laser (694 nm). | Usui78F061 |
| 5.36.24 | CH ₂ Cl ₂ | 1.6×10^9 *1.2 × 10° | 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]. | Usui78F061 |
| 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 × 10 ⁷ (*7.0 × 10 ⁷) dm ³ mol ⁻¹ | Brew74F646 |
| 5.36.26 | CHCl ₃ | $(3.6 \pm 0.5) \times 10^8$ | | rt | Ad-8 | s^{-1} [A3.16]. S = MB, dye laser | Brew74F646 |
| 5.36.27 | CHCl ₃ | 7.0×10^8 | | 25 | Ad-5 | $(610 \text{ nm}).^a$ S = MB, ruby laser | Usui78F061 |
| 5.36.28 | CHCl ₃ | 9.0×10^8 | 1.0×10^{-5} | 25 | Ad-15 | (694 nm). S = MB. k derived using $k_d = 9.0 \times 10^3$ s^{-1} [1.5.2]. | Usui78F061 |
| 5.36.29 | CCl₄ | $(2.6 \pm 0.4) \times 10^8$ | | 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]. | Usui78F061 |

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

| No. Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $(\beta = k_{d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|--|--|---|----------|-----------------------|--|------------|
| 5.36.31 | CCl₄ | $(8.0 \pm 2.4) \times 10^8$ | | rt | Ld-13 | $S = ? k \text{ derived using } k_d = 3.6 \times 10^1 \text{ s}^{-1}$. [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]. | Brew74F646 |
| 5.36.33 | EtOH | $(1.02 \pm .02) \times 10$ | 99 | 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]. | Usui78F061 |
| 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 $k_D = 5.1 \times 10^{-5} \text{ s}^{-1}$ at [DPBF] = 1.7 × 10 ⁻⁵ mol dm ⁻³ . | Youn73F014 |
| 5.36.36 | CHCl ₂ C | $H_3 6.0 \times 10^8$ | | 25 | Ad-5 | S = MB, ruby laser (694 nm). | Usui78F061 |
| 5.36.37 | CHCl ₂ C | $H_3 1.0 \times 10^9$ | 1.5×10^{-5} | 25 | Ad-15 | S = MB. k derived using $k_d = 1.5 \times 10^4$ s ⁻¹ [1.13]. | Usui78F061 |
| 5.36.38 | CH₂F- CH₂OH | $(5.1 \pm 3.9) \times 10^8$ | | rt | Ad-8 | S = MB, dye laser (610 nm). Solvent contained 1% MeOH. ^a | Brew74F646 |
| 5.36.39 | CHCl₂- CH₂OH | $(5.7 \pm 1.1) \times 10^8$ | | rt | Ad-8 | S = MB, dye laser (610 nm). ^a | Brew74F646 |
| 5.36.40 | CCl ₃ - CH ₂ OH | $(2.7 \pm 1.2) \times 10^8$ | | rt | Ad-8 | S = MB, dye laser (610 nm). Solvent contained 1% MeOH. ^a | Brew74F646 |
| 5.36.41 | CF ₃ CH ₂ O | OH 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 | CF₃CH₂C | $OH k_r = 1.2 \times 10^8$ | | 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 ₃ CH ₂ C | OH $(6.0 \pm 1.3) \times 10^8$ | | rt | Ad-8 | S = MB, dye laser (610 nm). Solvent contained 1% MeOH. ^a | Brew74F646 |
| 5.36.44 | CH₃CN | 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 | CH₃CN | $k_r = 1.1 \times 10^9$ *3.9 × 10 ⁸ | | rt | Ad-17 A'd (sep) | | Brew74F646 |
| 5.36.46 | CH ₃ CN | $(6.6 \pm 0.7) \times 10^8$ | | 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). | Usui78F061 |
| 5.36.48 | CHCl ₂ - CHCl ₂ | 5.9 × 10 ⁸ | 1.4×10^{-5} | 25 | Ad-15 | · · · · · · · · · · · · · · · · · · · | Usui78F061 |

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

| No. Substrate (A) | Solvent /d | k mol ⁻¹ s ⁻¹ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|--|--|---|----------|-----------------------|---|-------------|
| 5.36.49 | CCl ₂ F- CCIF ₂ | $k_{\rm r}=4.0\times10^7$ | | rt | Ad-36 | $^{1}\text{O}_{2}$ * from Nd-YAG CW laser (1065 nm). Measured $(k_r/k_{\text{O}_2} \text{O}_2) = 1 \times 10^4 \text{ dm}^3 \text{ mol}^{-1}$. k_r derived using $k_{\text{O}_2} \text{O}_2 = 4 \times 10^3 \text{ s}^{-1}$ (based on gas phase value for k_{O_2} of $1.3 \times 10^3 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$). | Math.70F387 |
| 5.36.50 | CCl ₂ F- CClF ₂ | $(1.0 \pm 0.2) \times 10^9$ | | rt | Ad-5 | ¹ O ₂ * from pulsed Nd- YAG laser (1065 nm). | Math74F10 |
| 5.36.51 | CCl ₂ F- CClF ₂ | $k_{\rm r} = (1.7 \pm 0.6) \times 10^8$ | | rt | Ad-5 | $^{1}\text{O}_{2}^{*}$ from pulsed Nd-YAG laser (1065 nm). k_{r} derived using $k_{\text{A}} = 1.0 \times 10^{9} \text{ dm}^{3} \text{ mol}^{-1}$ $\text{s}^{-1} [5.36.50] \text{ and } k_{\text{O}2} = 2.7 \times 10^{3} \text{ dm}^{3} \text{ mol}^{-1}$ | Math74F10 |
| 5.36.52 | CCl ₂ F- CClF ₂ | $k_{\rm r}=7.6\times10^7$ | | rt | Ad-36 | s ⁻¹ [15.1.4]. ${}^{1}O_{2}$ * 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]. | Math74F10 |
| 5.36.53 | CCl ₂ F- CCIF ₂ | 1.02×10^{7} $k_{\rm r} = 1.0 \times 10^{7}$ $k_{\rm q} = 2.0 \times 10^{5}$ | 4.6 × 10 ⁻⁵ | 25 | Ad-34 | | Evan.76F417 |
| 5.36.54 | i-PrOH | 4.5×10^{8} | $(1.1 \pm 0.3) \times 10^{-4}$ | rt | Ad-15 | | Brew74F646 |
| 5.36.55 | i-PrOH | $k_{\rm r} = 6.1 \times 10^8$ *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 × 10° (*7.0 × 10°) dm³ 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) ₂ CO | 6.5×10^8 | $(4.8 \pm 1.3) \times 10^{-5}$ | rt | Ad-15 | | Brew74F646 |
| 5.36.58 | (Me) ₂ CO | $k_{\rm r} = 1.7 \times 10^9$ *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 × 10 ⁸ (*7.0 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [A3.16]. | Brew74F646 |
| 5.36.59 | (Me) ₂ CO | $(5.6 \pm 1.3) \times 10^8$ | | rt | Ad-8 | S = MB, dye laser (610 nm). ^a | Brew74F646 |
| 5.36.60 | epibromo- hydrin | $- (7.8 \pm 1.4) \times 10^{6}$ | 3 | 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 /c | k dm³ mol ⁻¹ s ⁻¹ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|------------|--|---|----------|-----------------------|--|------------|
| 5.36.61 | n-BuOH | $k_{\rm r} = 7.3 \times 10^8$ *5.0 × 10 ⁸ | $ \beta_{\rm 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 × 10 ⁻⁴ (*1.4 × 10 ⁻³) mol dm ⁻³ [5.30.5] and k_d = 5.2 × 10 ⁴ s ⁻¹ [1.24]. | Youn71F398 |
| 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 | Youn73F014 |
| 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 | $k_{\rm r} = 8.3 \times 10^8$ *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 × 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 | $k_{\rm r} = 6.1 \times 10^8$ *4.2 × 10 ⁸ | $ \beta_{\rm r} = 4.9 \times 10^{-5} \\ *7.2 \times 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 × 10 ⁻⁴ (*1.4 × 10 ⁻³) mol dm ⁻³ [5.30.5] and k_d = 3.0 × 10 ⁴ s ⁻¹ [1.25]. | Youn71F398 |
| 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 | Youn73F014 |
| 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 | $k_{\rm r} = 6.2 \times 10^8$ *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 × 10 ⁷ (*7.0 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [A3.16]. Solvent | Brew74F646 |
| 5.36.69 | ТНБ | $k_{\rm r} = 8.3 \times 10^8$ *7.8 × 10 ⁸ | | rt | Ad-17 A'd (sep) | contained 1% MeOH. ^a S = RB, A' = DPF. Measured $(k_r/k_r^{A'}) =$ 11.1. k_r derived using $k_r^{A'} = 7.5 \times 10^7$ $(*7.0 \times 10^7) \text{ dm}^3 \text{ mol}^{-1}$ $s^{-1} [A3.16].$ | 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 | $(1.21\pm0.16)\times10^9$ | $(2.4\pm0.8)\times10^{-5}$ | rt | Ad-8 | S = MB, dye laser (610 nm). ^a | Youn73F014 |
| 5.36.72 | dioxane | $k_{\rm r} = 3.1 \times 10^8$ *8.0 x 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 × 10 ⁷ (*7.0 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [43.16]. | 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 /c | k lm³ mol ⁻¹ s ⁻¹ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|-----------------------------------|--|---|----------|-----------------------|--|-------------|
| 5.36.74 | ethyl acetate | $k_{\rm r} = 3.5 \times 10^8$ *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 × 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 | Brew74F646 |
| 5.36.76 | C ₅ H ₅ N | $k_{\rm r}=9.2\times10^8$ | | rt | Ad-17 A'd | (610 nm). ^a 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 [43.17]. | Wils66F041 |
| 5.36.77 | C ₅ H ₅ N | $(2.1 \pm 0.3) \times 10^9$ | $(1.5 \pm 0.7) \times 10^{-5}$ | rt | Ad-8 | S = MB, dye laser (610 nm). ^a | Youn73F014 |
| 5.36.78 | C3H3N | $k_{\rm r} = 4.8 \times 10^8$ *5.5 × 10 ⁸ | | rt | Ad-17 A'd (sep) | (**To lin!). S = RB, A' = DPF. Measured (k_r/k_r^A) = 7.86. k_r derived using $k_r^{A'}$ = 6.1 × 10 ⁷ (**7.0 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [A3.16]. Solvent contained 1% MeOH. ^a | Brew74F646 |
| 5.36.79 | C₅H₅N | $(5.0 \pm 3.5) \times 10^8$ | | rt | A d-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 ₆ H 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 | C₀H ₁₁ OH | $k_{\rm r} = 6.5 \times 10^8$ *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 × 10 ⁷ (*7.0 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [A3.16]. Solvent contained 1% MeOH. ^a | Brew74F646 |
| 5.36.83 | C ₆ H ₁₁ OH | $(1.4 \pm 2.2) \times 10^8$ | | rt | Ad-8 | S = MB, dye laser (610 nm). Solvent contained 1% MeOH. | 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 | $k_{\rm r}=7.0\times10^8$ | $(6.0 \pm 0.5) \times 10^{-5}$ | 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]. | Stev74F312 |
| 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 $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. Solvent contained 1% MeOH.* | Brew74F646 |
| 5.36.87 | C ₆ H 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 ₆ H ₆ | 6.7×10^{8} | $(6.0 \pm 0.5) \times 10^{-5}$ | 25 | Ad-15 | S = self. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Stev74F649 |
| | | | | | | . []- | |

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 | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|----------------------|---|--|---|----------|-----------------------|--|-------------------------|
| 5.36.89 | C ₆ H ₆ | $k_{\rm r} = 6.6 \times 10^{\rm s}$ *5.0 × 10 ^s | | 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]. | Stev74F649 |
| 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 $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Merk.78E036 |
| 5.36.91 | C ₆ H 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. | Gorm78E26 |
| 5.36.92 | C ₆ H ₆ | 6.7×10^8 | 6.0×10^{-5} | 25 | Pa-15 | S = self. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Stev.79E106 |
| 5.36.93 | C ₆ H ₅ Br | 5.9×10^8 | $(2.2 \pm 0.7) \times 10^{-5}$ | rt | Ad-15 | | Brew74F646 |
| 5.36.94 | C ₆ H ₅ Br | $(5.4 \pm 1.3) \times 10^{-1}$ | 98 | 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. | Brew74F646 |
| 5.36.96 | methyl benzoate | $(4.2 \pm 3.3) \times 10^{-10}$ | 8 | rt | Ad-8 | S = MB, dye laser (610 nm). Solvent contained 1% MeOH. | Brew74F646 |
| 5.36.97 | MeOH/H; (1:1) v:v | 20 5.1×10° | 5.5×10^{-5} | rt | Ad-8 16 | contained 17% MeO11. $S = RB \text{ or } MB$, dye laser. k derived from β and $k_D = (3.7 \pm 1.2) \times 10^{-5} \text{ s}^{-1}$ at $[DPBF] = 1.7 \times 10^{-5}$ mol dm ⁻³ . | Youn78F014 |
| 5.36.98 | MeOH /glycol (1:1) v:v | 1.9 × 10° | 6.3×10^{-5} | rt | Ad-8 16 | mordin . S = MB or RB, dye laser. k derived from β ar $k_D = (1.6 \pm 0.1) \times 10^{-5}$ s ⁻¹ at [DPBF] = 1.9×10^{-5} mol dm ⁻³ . | Youn73F014 ad |
| 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 | $k_{\rm r}=3.3\times10^9$ | | rt | Ad-14 | | Foot.76R071 |
| 5.36.101 | (99:1) v:v | | | 25 | Ad-5 | S = MB, flash photolysis. | Furu.78E238 |
| 5.36.102 5.36.103 | (98:2) v:v | OH 4.8×10^8 COH 5.4×10^8 | | 25 25 | Ad-5 Ad-5 | S = MB, flash photolysis. S = MB, flash | Furu.78E238 Furu.78E238 |
| 5.36.103 | (97:3) v:v | | | 25 | Ad-5 | photolysis. $S = MB, flash$ | Furu.78E238 |
| 5.36.105 | (96:4) v:v | OH 6.0×10^{8} | | 25 | Ad-5 | photolysis. S = MB, flash photolysis. | Furu.78E238 |

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

| 140. 3 | ubstrate (A) | Solvent /d | $\frac{k}{\text{lm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|----------|---|--|---|---|--------------|-----------------------|--|-------------|
| 5.36.10 | 6 | CCl ₄ /MeC (94:6) v:v | OH $(2.5 \pm 0.2) \times$ | 108 | rt | Ad-8 | S = MB, dye laser (610 nm). ^a | Brew74F646 |
| 5.36.10 | 7 | ` ' | OH (2.6 \pm 1.0) \times | 108 | rt | Ad-8 | S = MB, dye laser (610 nm). ^a | Brew74F646 |
| 5.36.10 | 8 | , , | OH (2.6 \pm 0.2) \times | 108 | rt | Ad-8 | S = MB, dye laser (610 nm). ^a | Brew74F646 |
| 5.36.10 | 9 | | OH (2.6 \pm 0.4) \times | 108 | rt | Ad-8 | S = MB, dye laser (610 nm). ^a | Brew74F646 |
| 5.36.11 | 0 | , , | H $(3.0 \pm 0.5) \times$ | 108 | rt | Ad-5 | S = MB, flash photolysis. | Floo73F334 |
| 5.36.11 | 1 | | OH $(9.1 \pm 2.0) \times$ | $10^8(4.1 \pm 0.8) \times 10^{-1}$ | rt rt | Ad-8 | S = MB, dye laser $(610 \text{ nm})^a$ | Youn73F014 |
| 5.36.11 | 2 | | OH 1.9×10^9 | $(2.0 \pm 1.2) \times 10^{-1}$ | 5 rt | Ad-15 | S = MB. k derived using $k_d = 3.8 \times 10^4$ s ⁻¹ [1.49]. ^a | Brew74F646 |
| 5.36.11 | 3 | C ₆ H ₆ /Me((4:1) v:v | OH $k_{\rm r} = 1.0 \times 10$ | D ⁹ | rt | Ad-17 A'd (sep) | S = MB, A' = DPF. (k_r/k_r^A) unreported. ^a | Brew74F646 |
| 5.36.114 | 4 | C ₆ H ₅ Br /MeOH (4:1) v:v | 4.6×10^8 | $(9.3 \pm 5.1) \times 10^{-3}$ | rt rt | Ad-15 | S = MB. k derived using $k_d = 4.3 \times 10^4$ s ⁻¹ [1.50]. ^a | Brew74F646 |
| 5.36.11: | 5 | C ₆ H ₅ Br /MeOH (4:1) v:v | $(7.0 \pm 1.3) \times 10^8$ | $(6.2 \pm 1.0) \times 10^{-1}$ | rt . | Ad-8 | $S = MB$, dye laser $(610 \text{ nm})^a$ | Youn73F014 |
| | | | 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- dimethylisobenzo- furan $[R_1 = R_3 = -Ph,$ $R_5 = R_6 = -Me]$ | МеОН | $k_{\rm r} = 5.24 \times 10^8$ *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 $\phi_{\rm isc} = 0.76$ [71M325]. | Olms.73F660 |
| 5.38 | 1,3,4,7-tetra- phenylisobenzo- furan $[R_1 = R_3 = R_4 =$ $R_7 = -Ph]$ | МеОН | $k_{\rm r} = 6.62 \times 10^8$ *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 $\phi_{\rm isc} = 0.76$ [71M325]. | Olms.73F660 |
| 5.39 | 1,3,4,5,6,7-hexa- phenylisobenzo- furan $[\mathbf{R}_1 = \mathbf{R}_3 = \mathbf{R}_4 =$ | МеОН | $k_{\rm r} = 6.88 \times 10^8$ *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 $\phi_{\rm isc} = 0.76$ [71M325]. | Olms.73F660 |
| 5.40 | $R_5 = R_6 = R_7 = -2$ -phenylbenzo[b]-cyclopentadieno[e]-pyran | C_6H_6 | 7.8×10^{5} | $(5.4 \pm 0.6) \times 10^{-6}$ | rt | Ad-15 | S = self. k derived using $k_d = 4.2 \times 10^4$ s ⁻¹ [1.32]. | Timp78F438 |
| | C _e H _s | | | | | | · | , |
| | | | | COMPOUNDS | 5.41 – 5.44 | ·: | | |
| | | | | 5 N | 2 | | | |
| 5.41 | $1-t$ -butylpyrrole $[\mathbf{R}_1 = -(t-\mathbf{B}\mathbf{u})]$ | MeOH - | 3.9×10^{7} $*3.2 \times 10^{7}$ | 9.7 × 10 ⁻⁴ | rt | Od-? | $S = MB$. k derived using $k_d = 3.8 \times 10^4$ | Ligh.75F652 |
| | | (Me) ₂ CO | | 1.2×10^{-4} | | | $(*3.1 \times 10^4) \text{ s}^{-1} [1.22].$ | |

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

| No. S | ubstrate (A) | Solvent /c | $\frac{k}{\text{lm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | <i>t</i> /°C | Method | Comments | Ref. |
|--------|---|------------------------------|---|---|-----------------|--------|--|-------------|
| 5.42 | $2-t-butylpyrrole$ $[R_2 = -(t-Bu)]$ | МеОН | 1.1 × 10 ⁸ | 9.3 × 10 ⁻⁴ | rt | Od~? | S = RB. k derived using $k_d = *1.0 \times 10^5$ | Ligh.75F652 |
| 5.42.1 | | (Me) ₂ CO | 4.2×10^{7} $*3.4 \times 10^{7}$ | 9.0 × 10 ⁻⁴ | rt | Od-? | s^{-1} [1.3.6]. S = MB. k derived using $k_d = 3.8 \times 10^4$ (*3.1 × 10 ⁴) s^{-1} [1.22]. | Ligh.75F652 |
| 5.43 | $3-t$ -butylpyrrole $[\mathbf{R}_3 = -(t-\mathbf{B}\mathbf{u})]$ | МеОН | 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) ₂ CO | 2.9×10^{7} *2.4 × 10^{7} | 1.3×10^{-3} | rt | Od-? | S = MB. k derived using $k_d = 3.8 \times 10^4$ (*3.1 × 10 ⁴) s ⁻¹ [1.22]. | Ligh.75F652 |
| 5.44 | 2,5-dimethylpyrrol $[R_2 = R_5 = -Me]$ | е МеОН | 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 | CCl₄ | $(1.7 \pm 2.2) \times$ | 10 ³ | rt | A'd-8 | S = MB, A' = DPBF, dye laser (610 nm). | Youn.76F903 |
| 5.46 | 1,2-diphenyl-4 <i>H</i> -4-methylcyclopent dieno[b]quinoline | | 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]. | Timp78F438 |
| | C ₆ H ₅ | | | | | | | |
| 5.47 | quinoline | EtOH | $< 1 \times 10^9$ (est) | | 0 | Od-23 | S = MB, A' = DMF. No measurable effect. | Dall72F518 |
| 5.48 | Permanax 45 (CH ₃ CH ₃ CH ₃) n | 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 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ [5.29.12]. | Dall72F518 |
| 5.49 | imidazole | H ₂ O (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 | \ <u>\</u> / | H_2O | 2.0×10^7 | | rt | Od-19 | S = chlorophyll-a, | Barb.78A278 |
| | | (pH 7.0) | | | | | $Q = N_3^-$. 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 | |
| 5.49.2 | | H ₂ O (pH 7.0) | 2.9×10^7 | | rt | Od-19 | (1% by volume). S = chlorophyll-a, $Q = N_3^- k \text{ derived}$ using $k_Q = 2 \times 10^8$ dm³ 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. S | Substrate (A) | Solvent /c | k lm ³ mol ⁻¹ s ⁻¹ | $(\beta = k_{\rm d}/k)$ /mol dm ⁻³ | <i>t</i> /°C | Method | Comments | Ref. |
|--------|--|--|--|---|-----------------|--------|--|------------------|
| 5.49.3 | | H ₂ O (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 | Barb.78A278 |
| 5.49.4 | | H ₂ O (pH 7.0) | 3.6×10^7 | | rt | Od-19 | (5% by volume). S = hematoporphyrin, $Q = N_3^-$. k derived using $k_Q = 2 \times 10^8$ dm³ mol ⁻¹ s ⁻¹ [12.9.6]. S solubilized in triton X-100 micelles (1% by volume). | Barb.78A278 |
| 5.49.5 | | H ₂ O (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 N CH2CH2NH2 | H ₂ O (pH 7.1) | 2.8×10^{7} | | 25 | Od-19 | S = phenosafranine, Q = NaN ₃ . k derived usin $k_Q = 2.0 \times 10^8$ dm ³ mol ⁻¹ s ⁻¹ [12.9.6]. | Kral.78A360 g |
| 5.50.1 | , , , , , , , , , , , , , , , , , , , | H ₂ O | 2.0×10^8 | 2.5×10^{-3} | 25 | Ad-15 | S = MB. k derived using $k_d = 5.0 \times 10^5 \text{s}^{-1}$ [1.1]. | Usui78F061 |
| 5.50a | 4-methyl-3,5- dioxotriazolo- norbornane | C ₆ H ₆ /MeOH (3:1) v:v | $< 3 \times 10^5$ (est) | | 25 | A'd-20 | S=RB. A' = cyclohexene k estimated using $\beta_{A'} = 3.1 \text{ mol dm}^{-3}$ [2.54.3] and $k_d =$ | . Kret.78F586 |
| | CH3-N | | | | | | $6.25 \times 10^4 \mathrm{s}^{-1}$ | |
| 5.51 | 2,5-diphenyloxaz $c_{e^{H_5}} _{N}^{O} _{N}^{C_{e^{H_5}}}$ | ole H ₂ O/D ₂ O (1:1) Mole % | $\begin{array}{c} 1.6 \times 10^8 \\ \text{(est)} \end{array}$ | 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. | Usui78F061 |
| 5.51.1 | | | $0.1.6 \times 10^8$ H (est) | 1.6×10^{-3} | 25 | Ad-15 | S = MB. k estimated using $k_d = 2.58 \times 10^5$ s ⁻¹ (calc). | Usui78F061 |
| 5.52 | phenoxazine | C ₆ H ₅ Br | 1.0×10^7 H (est) | | rt | A'd-23 | S = A' = Rub. k estimated using $k_{A'}$ = $4 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 4.89 \times 10^4 \text{ s}^{-1}$ (calc). | Rose77F240 |

^aThe errors reported on k or β are 90 % confidence limits.

^bThis 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 | $k / dm^3 \text{ mol}^{-1} \text{ s}^{-1}$ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|------|---|--|--|---------------------------------------|-------------|-------------|---|-----------|
| | C: | Note: k rep | resents the overall rate | constant unless k_r (e | chemical re | action rate | constant) | |
| | or | $k_{\rm q}$ (quench | ing rate constant) is sp | ecified; $k_{ m d}$ is the rate | constant fo | | | |
| .1 | ethylamine C ₂ H ₅ NH ₂ | CCl ₂ F- CClF ₂ | $(3.1 \pm 0.6) \times 10^4$ (est) | | 23 | | $^{1}O_{2}^{*}$ 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 | Math.72F5 |
| .2 | propylamine | CHCl ₃ | $(2.3 \pm 0.3) \times 10^5$ | | rt | | $mol^{-1} s^{-1}$ (gas phase value [71E034]). S = A' = Rub. | Monr77F48 |
| | CH ₃ CH ₂ CH ₂ NH ₂ | | | | | | 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]. | |
| .3 | isopropylamine CH ₃ CH(CH ₃)NH ₂ | МеОН | 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]. | Mart72F51 |
| .3.1 | | MeOH | 5.3 × 10 ⁴ | 1.87 | rt | | S = RB, A' = DPBF. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. | Youn73E |
| .3.2 | | МеОН | 5.0 × 10 ⁴ | 2.02 | rt | | S = RB, A' = DPBF. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. | Youn73E |
| .4 | butylamine CH ₃ (CH ₂) ₂ CH ₂ NH ₂ | CHCl ₃ | $(2.4 \pm 0.3) \times 10^5$ | | rt | | 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]. | Monr77F48 |
| .4.1 | | EtOH | $< 1 \times 10^9$ (est) | | 0 | | S = MB, A' = DMF. No measurable effect. | Dall72F51 |
| .5 | isobutylamine CH ₃ CH(CH ₃)CH ₂ N | CHCl ₃ NH ₂ | $(4.1 \pm 0.5) \times 10^5$ | | rt | | 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]. | Monr77F48 |
| .6 | t-butylamine CH ₃ C(CH ₃) ₂ NH ₂ | МеОН | 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]. | Mart72F51 |
| .6.1 | | МеОН | 7.4×10^{5} | 1.36×10^{-1} | rt | A'd-16 | S = RB, A' = DPBF k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Youn73E |
| .7 | cyclohexylamine $C_6H_{11}NH_2$ | МеОН | 8.9×10^4 | 1.12 | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Youn73E |
| .8 | benzylamine C ₆ H ₅ CH ₂ NH ₂ | МеОН | 2.9×10^{5} | 3.44×10^{-1} | rt | A'd-16 | $k_{\rm d} = 1.0 \times 10^5 {\rm s}^{-1}$ [1.3.6]. | Youn73E |
| .8.1 | | МеОН | 1.2×10^5 | 8.1×10^{-1} | rt | | S = MB, A' = DPBF. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. ^a | Mart72F51 |
| .8.2 | | EtOH | $< 1 \times 10^9$ (est) | | 0 | | S = MB, $A' = DMF$. No measurable effect. | Dall72F51 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|---|---|--|---------------------------------------|----------|--------|--|-------------|
| .9 | 2-phenyl- ethylamine C ₆ H ₅ CH ₂ CH ₂ NH ₂ | МеОН | 6.5 × 10 ⁵ | 1.54 × 10 ⁻¹ | rt | | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6].$ | Youn73E0 |
| 5.9.1 | 0 3 2 22 | 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 |
| 5.10 | 3-phenylpropyl- amine C ₆ H ₅ CH ₂ CH ₂ CH ₂ N | 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]. | Mart72F519 |
| .10.1 | | MeOH | 7.6×10^4 | 1.32 | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6].$ | Youn73E0 |
| 5.11 | 4-phenylbutyl- amine C ₆ H ₅ CH ₂ (CH ₂) ₂ CH | MeOH | 1.0×10^{5} | 9.8 × 10 ⁻¹ | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6].$ | Youn73E0 |
| .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]. | Mart72F519 |
| .12.1 | | МеОН | 2.1×10^6 | 4.77×10^{-2} | rt | | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Youn73E0 |
| .12.2 | | CHCl ₃ | $(1.5 \pm 0.2) \times 10^7$ | | rt | | 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 |
| .12.3 | | CCl ₂ F- CClF ₂ | $(5.7 \pm 0.9) \times 10^5$ (est) | | 23 | A'd-37 | In mol s [3.63.5]. $^{1}O_{2}$ * 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 |
| .12.4 | | C ₆ H ₆ /MeOH (3:1) v:v | 2.4 × 10 ⁶ | | 25 | A'd-20 | S = RB, A' = cyclohexene. k derived using $\beta_{A'} = 3.1 \text{ mol dm}^{-3}$ [2.54.3] and $k_d = 6.25 \times 10^4 \text{ s}^{-1}$. | Kret.78F586 |
| .13 | dipropyl- amine (CH ₃ CH ₂ CH ₂) ₂ NH | 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 |
| .14 | diisopropyl- amine ((CH ₃) ₂ CH) ₂ NH | 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 |
| 5.15 | tetrahydro- pyrrole | МеОН | 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].* | Mart72F519 |

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

| No. 5 | Substrate (A) | Solvent | /dm³ mol-1 s-1 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | d Comments | Ref. |
|--------|---|--|---|---------------------------------------|----------|--------------|---|------------|
| 6.15.1 | | МеОН | 2.4 × 10 ⁶ | 4.2×10^{-2} | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Youn73E06 |
| | | | COMPOUND | S 6.16 - 6.18 : | | | | |
| | | | 5 4 | √ 3 | | | | |
| 6.16 | piperidine | МеОН | 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]. | Mart72F519 |
| 6.16.1 | | МеОН | 1.0×10^{6} | 9.8×10^{-2} | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Youn73E06 |
| 6.16.2 | | CHCl ₃ | $(5.8 \pm 0.6) \times 10^6$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_d = 1.67 \times 10^4 \text{ s}^{-1}$ [1.5] and $k_{A'} = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3]. | Monr77F486 |
| 5.17 | 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 $k_{A'} = 5.3 \times 10^7$ $dm^3 \text{ mol}^{-1}$ s^{-1} [3.63.3]. | Monr77F486 |
| 5.18 | 2,2,6,6- tetramethyl-4- hydroxypiperidine $[R_2 = R_2 = R_6 =$ | CHCl ₃ | $< 2.0 \times 10^{5}$ (est) | | rt | A'd-33 | S = A' = Rub. No measurable effect. | Monr77F486 |
| 5.18.1 | $R_6 \approx -Me, R_4 = -1$ | OH] C ₆ H ₆ /EtOH (8:1) v:v | 5 × 10 ⁵ | | 22 | A'd-23 | S = RB, A' = Tetr. $k 	ext{ derived using } k_{A'} = 7 \times 10^7 	ext{ dm}^3 	ext{ mol}^{-1} 	ext{ s}^{-1}$ and $k_d = 3 \times 10^4 	ext{ s}^{-1}$. | Ivan75F445 |
| 5.18.2 | | C ₆ H ₆ /EtOH (8:1) v:v | $k_{\rm r} = 2.9 \times 10^3$ *4.9 × 10 ² | | 22 | Pa-17 A'd | and $k_d = 3 \times 10^{-5}$. S = RB, A' = Tetr, P = nitroxy radicals. Measured $(k_r/k_r^{A'}) =$ $4.1 \times 10^{-5} k_r$ derived using $k_r^{A'} = 7 \times 10^7$ $(*1.2 \times 10^7) \text{ dm}^3 \text{ mol}^{-1}$ $s^{-1} [A3.13].$ | Ivan75F445 |
| 5.19 | di(2-hydroxyethyl)- methylamine CH ₃ N(CH ₂ CH ₂ OH) | | $(2.1 \pm 0.3) \times 10^7$ | | rt | A'd-33 | S = A' = Rub, k derived using $k_d = 1.67 \times 10^4$ s ⁻¹ [1.5] and $k_{A'} = 5.3 \times 10^7$ | Monr77F486 |
| 5.20 | N,N-dimethyl- formamide HCON(CH ₃) ₂ | EtOH | $k_{\rm r}=3.0\times10^2$ | | rt | Pa-19 | dm³ mol ⁻¹ s ⁻¹ [3.63.3]. 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. | Zolo75F655 |

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

| No. Subst | trate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-----------|--|--|--|---------------------------------------|----------|--------------|---|-------------|
| but | N-dimethyliso- tenylamine $(H_3)_2C = CHN(C$ | 0 0 | $k_{\rm r}=3.1\times10^8$ | | 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [43.2]. | Foot75F656 |
| 6.21.1 | | C ₆ H ₆ /Me ₂ SO (4:1) v:v | $k_{\rm r}=3.2\times10^8$ | | 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [43.2]. | Foot75F656 |
| 6.21.2 | | C ₆ H ₆ /Me ₂ SO (3:2) v:v | $k_{\rm r}=2.3\times10^8$ | | 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [43.2]. | Foot75F656 |
| 6.21.3 | | C ₆ H ₆ /Me ₂ SO (1:4) v:v | $k_{\rm r}=2.7\times10^8$ | | 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [43.2]. | Foot75F656 |
| 6.21.4 | | C ₆ H ₆ /CH ₃ CN (4:1) v:v | $k_{\rm r}=2.3\times10^8$ | | 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [43.2]. | Foot75F656 |
| 5.21.5 | | C ₆ H ₆ /CH ₃ CN (1:19) v:v | $k_{\rm r}=2.8\times10^8$ | | 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 × 10 ⁷ dm³ mol ⁻¹ s ⁻¹ [43.2]. | Foot75F656 |
| 6.21.6 | | C ₆ H ₆ /pentane (1:19) v:v | $k_{\rm r}=2.1\times10^8$ | | 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 × 10 ⁷ dm³ mol ⁻¹ s ⁻¹ [43.2]. | Foot75F656 |
| 5.21.7 | | C ₆ H ₆ /MeOH (3:7) v:v | $k_{\rm r}=8.7\times10^7$ | | 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 × 10 ⁷ dm³ mol ⁻¹ s ⁻¹ [43.2]. | Foot75F656 |
| 6.21.8 | | C ₆ H ₆ /MeOH (1:19) v:v | $k_{\rm r}=6.6\times10^7$ | | 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 × 10 ⁷ dm³ mol ⁻¹ s ⁻¹ [43.2]. | Foot75F656 |
| | methylamine H ₃) ₃ N | МеОН | 1.5×10^7 | 6.69×10^{-3} | rt | A'd-16 | S = MB, A' = DPBF. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. ^a | Mart72F519 |
| | ethylamine ₂ H ₅) ₃ N | МеОН | 1.3×10^7 | 7.6×10^{-3} | rt | A'd-16 | S = RB, A' = DPBF. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. | Youn.72F514 |
| 6.23.1 | | МеОН | 7.4×10^6 | 1.35×10^{-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 |
| 6.23.2 | | МеОН | 1.0×10^7 | 9.7 × 10 ⁻³ | rt | A'd-16 | $k_{\rm d} = 1.0 \times 10^5 \rm s^{-1}$ $k_{\rm d} = 1.0 \times 10^5 \rm s^{-1}$ [1.3.6]. | Youn73E0 |

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

| No. S | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t ∕°C | Method | d 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 $k_A = 5.3 \times 10^7$ | Monr77F4 |
| 6.23.4 | | CCl ₂ F- CCIF ₂ | $(2.1 \pm 0.3) \times 10^6$ (est) | | 23 | A'd-37 | dm³ mol ⁻¹ s ⁻¹ [3.63.3]. $^{1}O_{2}$ * from Nd-YAG CW laser (1065 nm), A' = tetracyclone. Measured $(k/k_{O1}) = (1.6 \pm 0.3)$ x 10³. k estimated using $k_{O2} = 1.3 \times 10^{3}$ dm³ mol ⁻¹ s ⁻¹ (gas phase | Math.72F5 |
| 6.23.5 | | EtOH | $k_{\rm r}=2.7\times10^6$ | 3.1×10^{-1} | rt | Pa-19 | value [71E034]). $S = RB. k_r$ derived using $k_d = 8.3 \times 10^4 \text{ s}^{-1}$ [1.10] and $(k_q/k_r) =$ 9.3. | Zolo75F6 |
| 6.23.6 | | C ₅ H ₅ N | $k_{\rm r}=2.2\times10^7$ | 2.7×10^{-3} | rt | Od-14 27 | S = RB, A' = 2M2P. k derived using $k_d = *5.9 \times 10^4 \text{ s}^{-1}$ [1.29.1]. | Smit72F512 |
| 6.23.7 | | C₅H₅N | $k_{\rm q}=2.0\times10^8$ | 2.9 × 10 ⁻⁴ | rt | Od-14 27 | S = RB, A' = 2M2P. k derived using $k_d = *5.9 \times 10^4 \text{ s}^{-1}$ [1.29.1]. | Smit72F512 |
| 6.23.8 | | C ₅ H ₅ N | 1.4×10^8 | 4.2 × 10 ⁻⁴ | rt | Od-20 | S = RB, A' = 2M2P. k derived using $k_d = *5.9 \times 10^4 \text{ s}^{-1}$ [1.29.1]. | Smit72F512 |
| 5.24 | diethyl(2- hydroxyethyl)amine (C ₂ H ₅) ₂ NCH ₂ CH ₂ OH | CHCl ₃ | $(3.0 \pm 0.3) \times 10^7$ | | rt | A'd-33 | k = Rub. k derived using $k_d = 1.67 \times 10^4$ s^{-1} [1.5] and $k_A = 5.3 \times 10^7$ $k_A = 5.3 \times 10^7$ $k_A = 5.3 \times 10^7$ | Monr77F48 |
| 6.25 | diethyl(2- methoxyethyl)amine (C ₂ H ₃) ₂ NCH ₂ CH ₂ OC | CHCI ₃ | $(3.8 \pm 0.4) \times 10^7$ | | rt | A'd-33 | 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]. | Monr77F48 |
| 6.26 | diethyl(2-cyano- ethyl)amine (C ₂ H ₅) ₂ NCH ₂ CH ₂ CN | CHCl ₃ | $(2.7 \pm 0.3) \times 10^7$ | | rt | A'd-33 | $k_{\rm d} = 1.67 \times 10^4$ $k_{\rm d} = 1.67 \times 10^7$ $k_{\rm d} = 1.63 \times 10^7$ $k_{\rm d} = 1.63 \times 10^7$ $k_{\rm d} = 1.63 \times 10^7$ | Monr77F48 |
| 5.27 | diethyl(7-amino- heptyl)amine (C ₂ H ₅) ₂ NCH ₂ (CH ₂) ₅ C | CHCl ₃ CH ₂ NH ₂ | $(6.1 \pm 0.7) \times 10^7$ | | rt | A'd-33 | of the first section of the section | Monr77F48 |
| 6.28 | tributylamine (CH ₃ (CH ₂) ₂ CH ₂) ₃ N | CHCl ₃ | $(5.8 \pm 0.6) \times 10^7$ | | rt | A'd-33 | differential form of the following $k_d = 1.67 \times 10^4$ s ⁻¹ [1.5] and $k_{A'} = 5.3 \times 10^7$ dm ³ mol ⁻¹ s ⁻¹ [3.63.3]. | Monr77F48 |

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

| No. | Substrate (A) | Solvent | $\frac{k}{\text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | 1 Comments | Ref. |
|------------------|---|--|---|--|----------|-----------------|--|--------------------------|
| 6.28.1 | | EtOH | $\leq 1 \times 10^9$ (est) | | 0 | Od-23 | S = MB, A' = DMF. No measurable effect. | Dall72F518 |
| 6.29 | di(2-hydroxy- ethyl)-t-butylamine (CH ₃) ₃ CN(CH ₂ CH ₂ | | $(1.1 \pm 0.2) \times 10^6$ | | - rt | A'd-33 | S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ $s^{-1} \{1.5\}$ and $k_{A'} = 5.3 \times 10^7$ | Monr77F486 |
| 6.30 | nicotine | МеОН | 4.4×10^{5} | 2.27×10^{-1} | 15 | Od-? | dm³ mol ⁻¹ s ⁻¹ [3.63.3]. 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 | С ₆ Н ₆ | 2.7×10^{7} | 1.47×10^{-3} | | Ad-15 | S = ZnTPP. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Herl.78F474 |
| 6.31.1 | Ĥ | MeOH /C ₆ H ₆ (2:1) | 4.0×10^{7} (est) | 2.02×10^{-3} UNDS $6.32 - 6.36$: | | Ad-15 | S = ZnTPP. k derived using $k_d = 8.0 \times 10^4$ s ⁻¹ (calc). | Herl.78F474 |
| | | | | s 2 3 | | | • | |
| 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 $k_d = 1.67 \times 10^4$ $s^{-1} [I.5]$ and $k_{A'} = 5.3 \times 10^7$ | 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 | dm ³ mol ⁻¹ s ⁻¹ [3.63.3] S = A' = Rub. k derived using $k_d = 1.67 \times 10^4$ s ⁻¹ [1.5] and $k_A = 5.3 \times 10^7$ | Monr77F486 |
| 6.33.1 6.33.2 | | CH ₂ Cl ₂ CH ₂ Cl ₂ | 5×10^{7} 8.6×10^{7} | 1.4×10^{-4} | 22 rt | A'd-? A'd-19 | dm³ mol ⁻¹ s ⁻¹ [3.63.3]. Method not given. S = A' = Tetr. k derived using $k_{A'} = 3.0 \times 10^7 \text{ dm}^3 \text{ mol}^{-1}$ | Ivan75F44 Byst.75F654 |
| 6.33.3 | | | OH $k_r = 2.3 \times 10^3$ *4.0 × 10 ² | | 22 | Pa-17 A'd | s ⁻¹ [3.62]. 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 × 10 ⁷ (*1.2 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [43.13]. | Ivan75F44 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol-1 s-1 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Metho | d Comments | Ref. |
|--------|--|--|-----------------------------|---------------------------------------|----------|--------|---|-------------|
| 6.34 | N-(2-hydroxy- ethyl)-2,2,6,6- tetramethyl- piperidine $[R_2 = R_2 = R_6 =$ $R_6 = -Me, R_1 =$ $-CH_2CH_2OH]$ | CHCl ₃ | < 2 × 10 ⁵ (est) | | rt | Ad'-33 | S = A' = Rub. No measurable effect. | Monr77F48 |
| 5.35 | N-(2-acetoxy- ethyl)-2,2,6,6- tetramethyl- piperidine $[R_2 = R_2 = R_6 =$ $R_6 = -Me, R_1 =$ $-CH_2CH_2OCOCH_2$ | CHCl ₃ | < 2 × 10 ⁵ (est) | | rt | A'd-33 | S = A' = Rub. No measurable effect. | Monr77F48 |
| 5.36 | 1-cyclohexyl- piperidine $[R_1 = -C_6H_{11}]$ | 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 |
| 5.37 | N -allylurea $CH_2 = CHCH_2NHCC$ | H ₂ O (pH 7.1) ONH ₂ | < 2 × 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 |
| 5.38 | quinuclidine | МеОН | 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]. | Youn73E |
| .39 | piperazine | МеОН | 1.4×10^6 | 7.3×10^{-2} | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Youn73E |
| .40 | 1,4-diazabi- cyclo[2.2.2]octane (DABCO) | МеОН | 1.5×10^7 | 6.5×10^{-3} | rt | P'a-20 | S = ZnTPP, A' = 2M2P. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Foot72F02 |
| .40.1 | Ň | МеОН | 8.1 × 10 ⁶ | 1.23×10^{-2} | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ | Youn.72F51 |
| .40.2 | | CHCl ₃ | $(5.2 \pm 0.6) \times 10^7$ | | rt | A'd-33 | [1.3.6]. 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]. | Monr77F48 |
| 5.40.3 | | CCl ₄ | $(7.0 \pm 2.1) \times 10^6$ | | rt | Ld-13 | am mol 's '[3.63.3]. S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ [1.8.3]. | Kras79A010 |
| 5.40.4 | | CS ₂ | 2.9×10^7 | 1.7×10^{-4} | rt | P'a-20 | S = ZnTPP, A' = 2M2P. k derived using $k_d = 5.0 \times 10^3 \text{ s}^{-1}$ [1.9]. | Foot72F02 |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | d Comments | Ref. |
|-------------------|---|--|---------------------------------------|----------|--------|--|-------------|
| 6.40.5 | EtOH | 1.4 × 10 ⁷ | | rt | Ad-23 | S = RB, A' = hexamethylenedithiocarbamate. Measured $k_{\rm A'}/(k_{\rm d} + k[{\rm A}]) = 58$ at [A] = 4.48 \times 10 ⁻⁴ mol dm ⁻³ . k derived using $k_{\rm A'} = 2.7 \times 10^8$ dm ³ mol ⁻¹ s ⁻¹ [11.42] and $k_{\rm d} = *7.9 \times 10^4$ s ⁻¹ [1.10.3]. | Yama72F11 |
| 6.40.6 | EtOH | $\leq 1 \times 10^9$ (est) | | 0 | Od-23 | S = MB, A' = DMF. No measurable effect. | Dall72F518 |
| 6.40.7 | EtOH | 3.11×10^{7} (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 |
| 6.40.8 | n-BuOH | 4.5×10^{6} | 1.15×10^{-2} | rt | A'd-16 | $k_{\rm d} = 5.2 \times 10^4 {\rm s}^{-1}$ [1.24]. | Youn.72F514 |
| 6.40.9 | C ₅ H ₅ N | 2.6 × 10 ⁸ | 2.3×10^{-4} | rt | Od-20 | $k_{\rm d} = *5.9 \times 10^4$ $k_{\rm d} = *5.9 \times 10^4$ $k_{\rm d} = *5.9 \times 10^4$ | Smit72F512 |
| 6.40.10 | C ₅ H ₅ N | 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 |
| 5.40.11 | C5H5N | $(3.1 \pm 2.0) \times 10^8$ | | rt | A'd-23 | S = A' = Rub. k derived using $k_{A'} = 4 \times 10^7 \text{ dm}^3$ $mol^{-1} \text{ s}^{-1} \text{ and}$ $k_d = *6.0 \times 10^4$ $\text{s}^{-1} [1.29.1].$ | Fahr74R11 |
| 5.40.12 | C ₆ H ₆ | 4.2×10^7 | 9.6 × 10 ⁻⁴ | rt | P'a-20 | S = ZnTPP, $A' = 2M2P$. k derived using $k_d = *4.0 \times 10^4 \text{ s}^{-1}$ [1.32.9]. | Foot72F028 |
| 5.40.13 | C ₆ H ₆ | 1.4×10^{7} | $(2.9 \pm 0.1) \times 10^{-3}$ | rt | | | Timp78F438 |
| 5.40.14 | C ₆ H ₅ CH ₃ | 1.9×10^8 | 2.1 × 10 ⁻⁴ (est) | rt | A'd~23 | $S = A' = \text{Rub. } \beta$ estimated using $\beta_{A'} = 9.1 \times 10^{-4} \text{ mol } \text{dm}^{-3} [3.63.25]. k$ derived using $k_d = 4.0 \times 10^4 \text{ s}^{-1} [1.36].$ | Ouan.68F285 |
| 5.40.15 | C ₆ H ₆ CH ₃ | 6.7×10^{8} (est) | | rt | | S = A' = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1} \text{ (calc)}$ and $k_{A'} = 1.7 \times 10^8$ dm³ mol ⁻¹ s ⁻¹ . | Zwei.75P063 |
| 5.40.16 | C₀H₅Br ¯ | 8.7×10^8 | 1.5 × 10 ⁻⁵ (est) | rt | | 1 O 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 /dm³ mol⁻¹ s⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | d Comments | Ref. |
|---|---|-----------------------------|---------------------------------------|----------|--------|--|--------------|
| 6.40.17 | C ₆ H ₅ Br | 2.6 × 10 ⁷ | | 0 | A'd-33 | $^{1}O_{2}$ * from microwave discharge, A' = Rub. Measured $k/[k_{d}/[A']] + k_{A'}] = 0.2$ 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]. | Guil.73F333 |
| 6.40.18 | o-C ₆ H ₄ Cl ₂ | 5.2 × 10 ⁶ (est) | 2.5×10^{-3} (est) | rt | A'd-23 | 1 O 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 $k_d(C_6H_3Br) = 1.3 \times 10^4$ 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 $k_d = 4.7 \times 10^7 \text{ s}^{-1} \{I(a).6.1\}$ and $k_{A'} = 7.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ . | Carl74F341 |
| 6.40.20 | C_6H_6 /MeOH (4:1) v:v | 1.6×10^7 | | 25 | | 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 . | Foot70F73 |
| 6.40.21 | CH ₂ Cl ₂ /MeOH /C ₅ H ₅ N (90:5:5) v:v:v | 3.3×10^7 (est) | | 25 | A'd-32 | $^{1}O_{2}^{*}$ from $(PhO)_{3}PO_{3}$ decomp., $A' = Rub$. k estimated using $k_{d} = 8 \times 10^{3} \text{ s}^{-1}$ and $k_{A'} = 7.3 \times 10^{7}$ dm ³ mol ⁻¹ s ⁻¹ . | Carl.,74F341 |
| 6.40.22 | CH ₂ Cl ₂ /MeOH /C ₃ H ₅ N (94:3:3) v:v:v | 3.3×10^{7} (est) | | 25 | A'd-32 | thin find s. ${}^{1}O_{2}* \text{ from } (PhO)_{3}PO_{3}$ decomp., A' = Rub. $k \text{ estimated using}$ $k_{A'} = 7 \times 10^{7} \text{ dm}^{3}$ $\text{mol}^{-1} \text{ s}^{-1} \text{ and } k_{d} = 7.3 \times 10^{3} \text{ s}^{-1}$. | Carl72F319 |
| 6.40.23 | <i>i</i> -octane /MeOH /C ₅ H ₅ N (94:3:3) v:v:v | 3.5×10^{7} (est) | | 25 | A'd-32 | $^{1}O_{2}^{*}$ from (PhO) ₃ PO ₃ decomp., A' = Rub. k estimated using $k_{A'}$ = 7×10^{7} dm ³ mol ⁻¹ s ⁻¹ and $k_{d} = 5.0 \times 10^{4}$ s ⁻¹ . | Carl72F319 |
| 6.40.24 | | 3.9×10^7 (est) | | 25 | A'd-32 | $^{1}O_{2}^{*}$ from $(PhO)_{3}PO_{3}$ decomp., $A' = Rub$. k estimated using $k_{d} =$ $4.7 \times 10^{4} \text{ s}^{-1}$ and $k_{A'} = 7.3 \times 10^{7}$ dm ³ mol ⁻¹ s ⁻¹ . | Carl74F341 |
| hexamethylene- tetramine N——————————————————————————————————— | МеОН | 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 |
| N —— CH ₂ 6.41.1 | МеОН | 2.2 × 10 ⁵ | 4.6 × 10 ⁻¹ | · rt | | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Youn73E06 |

 $^{^{}a}\beta$ 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 /dm³ mol⁻¹ s⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|--|---|--|---------------------------------------|----------|--------------|--|-------------|
| | | | resents the overall rate | | | | | |
| 7 1 | aniline | or k_q (quenchin | ng rate constant) is spec | ified; k_a is the rate | | | | D #45300 |
| 7.1 | C ₆ H ₅ NH ₂ | r | 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 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ [2.35.3]. | Pouy.71F29 |
| 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 × 10 ⁸ dm ³ | Dall72F518 |
| | IJ' | | | | | | $mol^{-1} s^{-1} [5.29.12].$ | |
| 7.3 | N-methylaniline C ₆ H ₅ NHCH ₃ | МеОН | 3.0×10^{7} | 3.4×10^{-3} | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6].* | Youn73E0 |
| 7.3.1 | | CCl ₂ F- CClF ₂ | $(3.8 \pm 0.3) \times 10^4$ (est) | | 23 | A'd-37 | 1 O ₂ * from Nd-YAG CW laser (1065 nm), A' = tetracyclone. Measured (k/k_{O2}) = $(2.9 \pm 0.2) \times 10^{1}$. | Math.72F51 |
| | | | | | | | k estimated using $k_{O2} = 1.3 \times 10^3 \text{ dm}^3$ mol ⁻¹ s ⁻¹ (gas phase value [71E034]). | |
| 7.4 | diphenylamine (C ₆ H ₅) ₂ NH | МеОН | 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 | | МеОН | 6.7×10^6 | 1.5×10^{-2} | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. ^a | Youn73E |
| 7.5 | 4,4'-di-I-octyl-diphenylamine CH ₃ C(CH ₃)CH ₂ C(CH ₃) ₅ NH CH ₃ C(CH ₃)CH ₂ C(CH ₃) ₃ | C ₆ H ₆ /Ett (8:1) v:v | OH 7.3 × 10 ⁶ (est) | | 22 | A'd-23 | S = RB, A' = Tetr, A" = Ni(II) dibutyldithiocar- bamate. k estimated using $k_{A''} = 1.6 \times 10^9$ dm³ mol ⁻¹ s ⁻¹ [10.17.12], $k_{A'} = 7 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ and $k_d = 3 \times 10^4$ s ⁻¹ (calc) | |
| 7.5.1 | | C ₆ H ₆ /Et ¹ (8:1) v:v | OH $k_{\rm r} = 2.6 \times 10^4$ *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 × 10 ⁷ (*1.2 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [A3.13]. | Ivan75F4 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|--|---------------------------------|--|---------------------------------------|----------|--------|---|-------------|
| | | | T | COMPOUNDS 7.6 | - 7.13 : | | | |
| | | | | N(CH ₃) ₂ | | | | |
| | | | | 3 3 | | 7 | | |
| 7.6 | N,N-dimethyl- aniline | МеОН | 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].* | Mart72F519 |
| 7.6.1 | | МеОН | 1.3×10^8 | $(7.6 \pm 0.9) \times 10^{-4}$ | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6].* | Youn73E00 |
| 7.6.2 | | МеОН | $(7.3 \pm 0.8) \times 10^7$ | | rt | A'd-8 | S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn73F014 |
| 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 | | CCl₂F− CClF₂ | $(2.0 \pm 0.4) \times 10^5$ (est) | | 23 | A'd-37 | $^{1}O_{2}^{*}$ from Nd-YAG CW laser (1065 nm), A' = tetracyclone. Measured $(k/k_{O2}) = (1.6 \pm 0.3) \times 10$ k estimated using $k_{O2} = 1.3 \times 10^{3}$ dm ³ mol ⁻¹ | Math.72F513 |
| 7.6.5 | | C ₅ H ₅ N | 1.0×10^{8} *1.9 × 10 ⁸ | 5.9 × 10 ⁻⁴ | rt | Od-20 | s ⁻¹ (gas phase value [71E034]). S = RB, A' = 2M2P. k derived using $\beta_{A'}$ = 4.3×10^{-2} mol dm ⁻³ and k_d = 3.1×10^4 | Smit75F166 |
| 7.7 | m-chloro-N,N-dimethylaniline | МеОН | 2.2×10^6 | 4.52×10^{-2} | rt | A'd-16 | (*5.9 × 10 ⁴) s ⁻¹ [1.29]. S = MB, A' = DPBF. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. ^a | Mart72F519 |
| 7.7.1 | $[R_3 = -Cl]$ | МеОН | 1.4×10^{7} | 7.15×10^{-3} | , rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. ^a | Youn73E06 |
| 7.7.2 | | МеОН | $(1.1 \pm 0.1) \times 10^7$ | | rt | A'd-8 | S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn74F64 |
| 7.8 | p -bromo- N , N - dimethylaniline $[R_4 = -Br]$ | МеОН | 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 | [4 - 22] | МеОН | 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]. ⁸ | Youn73E06 |
| 7.8.2 | | МеОН | $(1.7 \pm 0.4) \times 10^7$ | | rt | A'd-8 | S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn74F64 |
| 7.9 | p -methyl- N , N - dimethylaniline $[R_4 = -Me]$ | МеОН | 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 /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---|---------|--|---------------------------------------|----------|--------|---|------------|
| 7.9.1 | МеОН | 1.8 × 10 ⁸ | $(5.5 \pm 0.3) \times 10^{-4}$ | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6].* | Youn73E06 |
| 7.9.2 | МеОН | $(1.2 \pm 0.4) \times 10^8$ | | rt | A'd-8 | S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn74F64 |
| 7.10 p -cyano- N , N - dimethylaniline $[R_4 = -CN]$ | МеОН | 4.0×10^6 | 2.51×10^{-2} | rt | A'd-16 | S = MB, A' = DPBF. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. ^a | Mart72F51 |
| 7.10.1 | МеОН | 2.0×10^{6} | 5.0×10^{-2} | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. ^a | Youn73E06 |
| 7.10.2 | МеОН | $(5.7 \pm 0.1) \times 10^5$ | | rt | A'd-8 | S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn74F64 |
| 7.11 $p-(N,N-$ dimethylamino)- benzaldehyde $[R_4 = -CHO]$ | МеОН | 2.2 × 10 ⁶ | 4.58×10^{-2} | rt | A'd-16 | S = MB, A' = DPBF. k derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6].* | Mart72F519 |
| 7.11.1 | МеОН | 2.7×10^6 | 3.7×10^{-2} | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ | Youn73E06 |
| 7.11.2 | МеОН | $(1.2 \pm 0.6) \times 10^6$ | | rt | A'd-8 | [1.3.6]. ^a S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% | Youn74F644 |
| 7.12 m -methoxy- N,N -dimethyl-aniline $[R_3 = -OCH_3]$ | МеОН | 1.4×10^8 | 7.07 × 10 ⁻⁴ | rt | A'd-16 | confidence limit. S = MB, $A' = DPBF$. $kderived using k_d =*1.0 \times 105 s-1 [I.3.6].a$ | Mart72F519 |
| 7.12.1 | МеОН | 6.7×10^7 | $(1.5 \pm 0.4) \times 10^{-3}$ | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ | Youn73E06 |
| 7.12.2 | МеОН | $(4.8 \pm 0.4) \times 10^7$ | | rt | A'd-8 | [1.3.6]. ^a S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence | Youn74F64 |
| 7.13 p -methoxy- N,N -dimethyl-aniline $[R_4 = -OCH_3]$ | МеОН | 5.5×10^8 | 1.84 × 10 ⁻⁴ | rt | A'd-16 | limit. S = MB, $A' = DPBF$. $kderived using k_d =*1.0 × 105 s-1 [1.3.6].a$ | Mart72F519 |
| 7.13.1 | МеОН | 2.1×10^8 | $(4.7 \pm 1.1) \times 10^{-4}$ | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ | Youn73E06 |
| 7.13.2 | МеОН | $(1.8 \pm 0.4) \times 10^8$ | | rt | A'd-8 | [1.3.6]. ^a S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn74F64 |
| o-phenylenedi- amine | EtOH | 3.4 × 10° | | 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 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ [5.29.12]. | Dall72F518 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol-1 s-1 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|-----------------|-----------------------------|---------------------------------------|----------|--------|--|------------|
| 7.15 | 4,4'-diamino- biphenyl | ЕюН | 3.0 × 10° | | 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 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ [5.29.12]. | Dall72F518 |
| 7.16 | 1-isopropylamino- 4-phenylamino- benzene NHCH(CH ₃) ₂ | 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 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ [5.29.12]. | Dall72F518 |
| 7.16.1 | Nнс _в н ₅ I | i-octane | 3.3×10^8 (est) | | rt | A'd-23 | S = A' = Rub. k estimated using $k_d = 4 \times 10^4 \text{ s}^{-1}$ | Carl73P066 |
| 7.16.2 | 2 | i-octane | 2.1 × 10 ⁸ (est) | | 25 | A'd-23 | [1(a).6] and $k_{A'} = 7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. S = A' = Rub. k estimated using $k_d = 4.7 \times 10^4 \text{ s}^{-1}$ [1(a).6.1] and $k_{A'} =$ | Carl74F341 |
| 7.16.3 | ; | hexa- decane | 4.0 × 10 ⁸ (est) | | 25 | A'd-33 | 7.3 \times 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ . ¹ O ₂ * from microwave discharge, A' = Rub. k estimated using $k_d = 9.0 \times 10^4$ s ⁻¹ [1(a).7] and $k_{A'} =$ | Carl74F341 |
| 7.17 | 1-cyclohexylamino 4-phenylamino- benzene | EtOH | 5.9 × 10 ⁹ | | 0 | Od-23 | 7.3 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ . S = MB, A' = DMF. k derived using k_d = *7.9 × 10 ⁴ s ⁻¹ [1.10.3] and $k_{A'}$ = 5.3 × 10 ⁸ dm ³ mol ⁻¹ s ⁻¹ [5.29.12]. | Dall72F518 |
| 7.17.1 | ÑНС _Б Н _б | EtOH | 1.1×10^{10} | | 0 | | S = MB, A' = DMF. Measured $(k/k_{A'})$ = 47.4. k derived using $k_{A'}$ = *2.3 × 10 ⁸ dm ³ | Dall72F518 |
| 7.18 | 1-cyclohexyl- amino-4-phenyl- aminobenzene hydrochloride | EtOH | < 1 × 10° (est) | | 0 | Od-23 | $mol^{-1} s^{-1} [A3.15]$. S = MB, A' = DMF. No measurable effect. | Dall72F518 |
| | NH HCI | | | | | | | |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|-------------------------------|---|--|----------|--------|--|-------------|
| 7.19 | N,N',N'',N'''- tetramethyl- phenylene- diamine | МеОН | 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. | N(CH ₃) ₂ | МеОН | 6.7 × 10 ⁸ | $(1.5 \pm 0.3) \times 10^{-4}$ | rt | A'd-16 | S = RB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6].* | Youn73E |
| 7.19.2 | 2 | МеОН | $(1.0 \pm 0.2) \times 10^9$ | V. | rt | A'd-8 | S = MB, A' = DPBF, dye laser (610 nm). Error is a 95% confidence limit. | Youn74F6 |
| 7.20 | luminol | D ₂ O (pD 11.8) | $k_{\rm r} = (3 \pm 1) \times 10^7$ *1.8 × 10 ⁷ | $\beta_{\rm r} = (1.7 \pm 0.6) \times 10^{-3}$ | rt | A'd-35 | laser (1065 nm), A' = bilirubin. k derived using $k_d = 5 \times 10^4$ (*3.1 \times 10 ⁴) s ⁻¹ [1.2.3]. | Math.76F662 |

 $^{{}^{}a}\beta$ 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 /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|--|-----------------------------------|---|---------------------------------------|----------|----------------|--|-------------|
| | | | | ite constant unless k_r (| | | | |
| | | · | | pecified; $k_{\rm d}$ is the rate | | | | |
| 8.1 | α-alanine ο сн _з снс-он | D ₂ O (pD 8.1) | 2.0×10^{6} *1.2 × 10 ⁶ | | 22 | A'd-22 | $^{1}O_{2}^{*}$ directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using k_{d} = | Math75F14 |
| | NH ₂ | | | | | | $5.0 \times 10^4 (*3.1 \times 10^4)$ s ⁻¹ [1.2.3]. | |
| 8.1.1 | | H ₂ O/MeO | $H < 1 \times 10^7$ | | rt | A'd-5 | S = MB, A' = DPBF, | Nils72F516 |
| | | (1:1) v:v | | | | | ruby laser (694 nm). | |
| 8.2 | methionine O CH3 SCH2CH2CHC-OH NH2 | H ₂ O | 2.2×10^7 | 2.0×10^{-2} | 10 | Od-15 | S = MB. k derived using $k_d = *4.4 \times 10^5$ s ⁻¹ [<i>I.1.3</i>]. The mechanism of oxidation is not clear. | Weil65F029 |
| 3.2.1 | | H ₂ O (pH 6) | 8.4 × 10 ⁷ | 5.2×10^{-2} | 25 | Ad-14 | S = proflavin. β derived using $\phi_{\rm ISC}$ = 0.73. k derived using $k_{\rm d}$ = *4.4 \times 10 ⁵ s ⁻¹ [1.1.3]. | Jori.70F732 |
| 8.2.2 | | H ₂ O (pH 7) | 1.15 × 10 ⁷ *5.06 × 10 ⁶ | | rt | A'd-16 | S = RB, A' = DPF. Plots are nonlinear. Used slope as $[A] \rightarrow 0$. k derived using $k_d = 1 \times 10^6 (*4.4 \times 10^5)$ s^{-1} [1.1.3]. | Sysa.77F433 |
| 3.2.3 | | H ₂ O (pH 11) | $\leq 5.0 \times 10^{7}$ $\leq *2.2 \times 10^{7}$ | | rt | A 'd-16 | S = RB, $A' = DPF$. Plots are nonlinear. Used slope as $[A] \rightarrow 0$. k derived using $k_d = 1 \times 10^6 (*4.4 \times 10^5)$ s^{-1} [1.1.3]. | Sysa77F43 |
| 3.2.4 | | H ₂ O (pH 7.1) | 8.6×10^6 | | 25 | Od-19 | S = phenosafranine, $Q = \text{NaN}_3$. $k \text{ derived}$ $u \sin k_Q = 2.0 \times 10^8$ $d \text{m}^3 \text{ mol}^{-1} \text{ s}^{-1} [12.9.6].$ | Kral.78A360 |
| 3.2.5 | | D ₂ O (pD 8.1) | 3×10^{7} *2 × 10 ⁷ | | 22 | A 'd-22 | 'O ₂ * directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using k_d = 5×10^4 (*3.1 \times 10 ⁴) s ⁻¹ [1.2.3]. | Math75F1 |
| 3.2.6 | | D ₂ O (pD 7) | 3.3×10^{7} | | rt | A'd-16 | S = RB, A' = DPF. Plots are nonlinear. Used slope as $[A] \rightarrow 0$. k derived using k_d (unreported). | Sysa77F43. |
| 3.2.7 | | D ₂ O (pD 11) | 1.57×10^7 | | rt | A'd-16 | S = RB, A' = DPF. Plots are nonlinear. Used slope as $[A] \rightarrow 0$. k derived using k_d (unreported). | Sysa.77F433 |
| 3.2.8 | | H ₂ O/MeO (1:1) v:v | H 3×10 ⁷ | | rt | A'd-5 | S = MB, A' = DPBF, ruby laser (694 nm). | Nils72F516 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_{d}/k)$ /mol dm ⁻³ | <i>t</i> /°C | Method | Comments | Ref. |
|-------|---|-----------------------------------|---|---|-----------------|--------------|--|-------------|
| 8.2.9 | | H ₂ O/MeO (1:1) v:v | $H k_r = 5 \times 10^6$ | | 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], $k_{Td}^{A} =$ 3×10^8 dm ³ mol ⁻¹ s ⁻¹ , and $k_A = 3 \times 10^7$ dm ³ | Nils72F516 |
| 8.3 | CBZ-L-methionine methyl ester CH3SCH2CH2CH2-OCH3 NHCOCH2CeH5 | CHCl ₃ | $(1.4 \pm 0.2) \times 10^7$ | | rt | A'd-33 | mol ⁻¹ s ⁻¹ [8.2.8]. 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]. | Monr79A08 |
| 8.4 | arginine | H ₂ O (pH 7.1) | $\leq 1 \times 10^6$ (est) | | 25 | Od-19 | S = phenosafranine. No measurable effect. | Kral.78A360 |
| | CNHCH2CH2CH2CHC-OH | 4 | | | | | | |
| 8.5 | tyrosine OH OH CH2CHC-OH NH2 | H ₂ O | 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 OH CH ₂ CH ₂ NH ₂ | H ₂ O (pH 10) | $(2.8 \pm 0.5) \times 10^8$ $k_{\rm r} = 2.4 \times 10^8$ | | 25 | Ad-? | S = MB, A' = NaN ₃ . k and k_r by computer fit of rate parameters to experimental Φ versus [A] data. | Seel77F489 |
| 3.7 | histidine N CH2CHC-OH H NH-2 | H ₂ O | 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 [<i>I.1.3</i>]. | Sluy61F008 |
| 8.7.1 | | H ₂ O | 5.43 × 10 ⁹ | 9.2×10^{-5} | 25 | Ad-15 | S = MB. k derived using $k_d = 5.0 \times 10^{5}$ s ⁻¹ L μ | Usui78F061 |
| 3.7.2 | | H ₂ O | 1.3×10^{8} | 3.44 × 10 ⁻³ | 10 | Od-15 | $5.0 \times 10^5 \text{ s}^{-1}$ [1.1]. S = MB. k derived using $k_d = *4.4 \times 10^5 \text{ s}^{-1}$ [1.1.3]. The mechanism of oxidation is not clear. | Weil65F029 |
| 8.7.3 | | H ₂ O (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 ₂ O (pD 8.1) | 1.7×10^{8} *1.1 × 10 ⁸ | | 22 | A'd-22 | 1 O 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]. | Math75F14 |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|------------------------------|------------------------------------|--|---------------------------------------|----------|--------------|---|------------|
| 8.7.5 | | H ₂ O/MeO (1:1) v:v | H 5×10 ⁷ | | rt | A'd-5 | S = MB, A' = DPBF, ruby laser (694 nm). | Nils72F516 |
| 8.7.6 | | | $H k_r = 7 \times 10^6$ | | rt | Ad-17 A'd | S = MB, A' = DPBF, k_r measured relative to $k_r^{A'} = k_A \text{ (MeOH)} =$ $8 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ $[5.36.9], k_r \text{ derived}$ using $k_d = 2.9 \times 10^5$ $\text{s}^{-1} [I.38], k_{Td}^{A} =$ $1 \times 10^6 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1},$ and $k_A = 5 \times 10^7 \text{ dm}^3$ $\text{mol}^{-1} \text{ s}^{-1} [8.7.5].$ | Nils72F516 |
| 8.8 | tryptophan NH 0 CH2CH—C—OH | H ₂ O | 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 ₂ O (pD 8.1) | 9×10^{7} *5.9 × 10^{7} | | 22 | A'd-22 | $^{1}O_{2}$ * 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]. | Math75F14 |
| 8.8.2 | | МеОН | $(6.0 \pm 2.0) \times 10^6$ | | rt | A'd-5 | S = MB, $A' = DPBF$, ruby laser (694 nm). | Smit78A338 |
| 8.8.3 | | EtOH | $\leq 5.0 \times 10^6$ | | 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 | | | $4 (3.0 \pm 0.1) \times 10^7$ | | rt | A'd-5 | S = MB, A' = DPBF, ruby laser (694 nm). | Smit78A338 |
| 8.8.6 | | H ₂ O/MeOH (1:1) v:v | 14×10^7 | | rt | A'd-5 | S = MB, $A' = DPBF$, ruby laser (694 nm). | Nils72F516 |
| 8.8.7 | | H ₂ O/MeOI (1:1) v:v | $4k_r = 4 \times 10^6$ | | 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]. | Nils72F516 |
| 8.9 | superoxide dismutase | D ₂ O (pD 8.1) | 2.6×10^9 *1.6 × 10 ⁹ | | 22 | A'd-22 | $^{1}O_{2}$ * 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]. | Math75F14 |
| 8.9.1 | | D ₂ O (pD 8.1) | 8.2×10^8 *5.1 × 10 ⁸ | | 22 | A'd-22 | S = MB, A' = bilirubin. k derived using $k_d = 5.0 \times 10^4 (*3.1 \times 10^4)$ s^{-1} [1.2.3]. | Math75F14 |

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

| No. Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | , /°C | Method | Comments | Ref. |
|----------------------------------|------------------------------|---|---------------------------------------|-------|-------------|---|-------------|
| 8.10 apo-superoxide dismutase | D ₂ O (pD 8.1) | 2.5 × 10° *1.6 × 10° | | 22 | A'd-22 | $^{1}O_{2}$ * directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using k_{d} = 5.0×10^{4} (*3.1 × 10 ⁴) | Math75F14 |
| 8.10.1 | D ₂ O (pD 8.1) | 1.1 × 10 ⁹ *6.8 × 10 ⁸ | | 22 | A'd-22 | s ⁻¹ [1.2.3]. S = MB, A' = bilirubin. k derived using k_d = 5.0×10^4 (*3.1 × 10 ⁴) s ⁻¹ [1.2.3]. | Math75F14 |
| 8.11 carbonic anhydrase | D ₂ O (pD 8.1) | 8.0×10^{8} *5.0 × 10 ⁸ | | 22 | A'd-22 | $^{1}O_{2}$ * directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using k_{0} = 5.0×10^{4} (*3.1 \times 10 ⁴) s ⁻¹ [1.2.3]. | Math75F14 |
| 8.11.1 | D ₂ O (pD 8.1) | 6.5×10^8 *4.0 × 10 ⁸ | | 22 | A'd-22 | S = MB, A' = bilirubin. k derived using k_d = 5.0×10^4 (*3.1 × 10 ⁴) s ⁻¹ [1.2.3]. | Math75F14 |
| 8.12 lysozyme | H ₂ O (pH 5.9) | $k_{\rm q} = 3.5 \times 10^8$ $k_{\rm r} = 1.6 \times 10^7$ | | 20 | Ad-14 | S = acridine orange. $k_{\rm q}$ and $k_{\rm r}$ derived using $k_{\rm d} = 5 \times 10^5$ s ⁻¹ [1.1]. | Schm.72R08 |
| 8.12.1 | H ₂ O | $k_{\rm r}=1.3\times10^8$ | | rt | Ad-28 | S = eosin-Y. k_r derived using k_d = 5.0×10^5 s ⁻¹ [1.1]. | Kepk.73R04 |
| 8.12.2 | H ₂ O (pH 5.9) | $k_{\rm q} = 4.1 \times 10^8$ $k_{\rm r} = 2.9 \times 10^7$ | | 20 | Ad-14 28 | $S = \text{acridine orange.}$ $k_q \text{ and } k_r \text{ derived}$ | Schm.76F10 |
| 8.12.3 | D ₂ O (pD 5.9) | $k_{\rm q} = 3.3 \times 10^8$ $k_{\rm r} = 1.5 \times 10^7$ | | 20 | Ad-14 | s ⁻¹ [1.1]. S = acridine orange. k_q and k_r derived using $k_d = *3.1 \times 10^4$ s ⁻¹ [1.2.3]. | Schm.72R08 |
| 8.12.4 | D_2O | $k_{\rm r} = 2.5 \times 10^8$ *1.6 × 10 ⁸ | | rt | Ad-28 | S = eosin-Y. k_r derived using k_d = 5.0×10^4 (*3.1 × 10 ⁴) s ⁻¹ [1.2.3]. | Kepk.73R04 |
| 8.12.5 | D ₂ O (pD 8.1) | 1.5 × 10 ⁹ *9.3 × 10 ⁸ | | 22 | A'd-22 | $^{1}O_{2}*$ directly from CW Nd-YAG laser (1065 nm), A' = bilirubin. k derived using k_{d} = $5.0 \times 10^{4} (*3.1 \times 10^{4})$ s ⁻¹ [1.2.3]. | Math75F14 |
| 8.12.6 | D_2O | 7.8×10^8 | 4.0×10^{-5} | 18 | Ad-15 | S = 8-methoxypsoralen. k derived using k_d = $*3.1 \times 10^4$ s ⁻¹ [1.2.3]. | Popp.75F485 |
| 8.12.7 | D ₂ O (pD 5.9) | $k_{\rm q} = 5.9 \times 10^{8}$ *3.7 × 10 ⁸ $k_{\rm r} = 4.7 \times 10^{7}$ *2.9 × 10 ⁷ | | 20 | Ad-14 28 | S = acridine orange. $k_{\rm q}$ and $k_{\rm r}$ derived using $k_{\rm d} = 5.0 \times 10^4$ (*3.1 × 10 ⁴) s ⁻¹ [1.2.3]. | Schm.76F10 |
| 8.13 trypsin | H ₂ O (pH 8.0) | 7.1 × 10 ⁹ | 7.0 × 10 ⁻⁵ | 15 | Pa-15 | S = MB and FMN. k derived using k_d = 5.0×10^5 s ⁻¹ [<i>I.I</i>]. 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 /dm³ 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 9.1 – 9.5:

| 9.1 | diazodiphenyl- methane (DDM) | МеОН | 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 | | Beth.77F113 |
| 9.1.2 | | CHCl ₃ | $k_{\rm r} = 1.1 \times 10^9$ *5.7 × 10 ⁸ | | rt | Ad-17 A'd | _ | Beth.77F113 |
| 9.1.3 | | CH ₃ CN | 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 ₃ CN | $k_r = 1.4 \times 10^9$ *3.8 × 10 ⁸ | | rt | Ad-17 A'd | | Beth.77F113 |
| 9.1.5 | | CH ₃ CN | $k_{\rm r} = 2.4 \times 10^9$ *6.5 × 10 ⁸ | | rt | Ad-17 A'd | $^{1}O_{2}*$ from (PhO) ₃ PO ₃ decomp., A' = DMA. Measured $(k_{r}/k_{r}^{A'})$ = 13.9. k_{r} derived using $k_{r}^{A'}$ = 1.7 × 10 ⁸ (*4.7 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [43.10]. | Beth.77F113 |
| 9.2 | diazo(4-bromo- phenyl)phenyl- methane [R = -Br] | CH ₃ CN | For more relative $k_r = 9.1 \times 10^8$ *3.8 × 10 ⁸ | e rates see 9.2- | 4, 9.4.3, rt | 9.5, 9.5.1. Ad-17 A'd | S = MB, A' = DDM. Measured $(k_r/k_r^{\Lambda'})$ = $(6.48 \pm 0.32) \times 10^{-1}$. k_r derived using $k_r^{\Lambda'}$ = 1.4×10^9 (*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 ₃ CN | $k_{\rm r} = 2.0 \times 10^9$ *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 × 10° (*5.9 × 108) dm³ mol ⁻¹ s ⁻¹ [A3.18]. | Beth.77F113 |
| 9.4 | diazodi(4-chloro- phenyl)methane [R = R' = -Cl] | МеОН | $k_{\rm r} = 3.8 \times 10^8$ *3.4 × 10 ⁸ | | rt | Ad-17 A'd | Measured $(k_r/k_r^A) = 0.577 \pm 0.038$. 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. 5 | Substrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|---|--------------------|--|---------------------------------------|----------|--------------|---|-------------|
| 9.4.1 | | CH ₃ CN | 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 ₃ CN | $k_{\rm r} = 7.3 \times 10^8$ *2.0 × 10 ⁸ | | rt | Ad-17 A'd | | Beth.77F113 |
| 9.4.3 | | CH ₃ CN | $k_{\rm r} = 7.5 \times 10^8$ *3.2 × 10 ⁸ | | rt | Ad-17 A'd | | Beth.77F113 |
| 9.5 | diazodi(4-methyl- phenyl)methane [R = R' = -Me] | - МеОН | $k_{\rm r} = 9.4 \times 10^8$ *8.3 × 10 ⁸ | | rt | Ad-17 A'd | | Beth.77F113 |
| 9.5.1 | | CH ₃ CN | $k_{\rm r} = 2.3 \times 10^9$ *9.7 × 10 ⁸ | | rt | Ad-17 A'd | | Beth.77F113 |
| 9.6 | 9-diazofluorene | МеОН | 3.3 × 10 ⁸ *2.4 × 10 ⁸ | $(4.2 \pm 0.7) \times 10^{-4}$ | rt | Ad-15 | | 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 | $k_{\rm r} = 6.8 \times 10^7$ *3.5 × 10 ⁷ | | rt | Ad-17 A'd | $^{1}O_{2}^{*}$ from (PhO) ₃ PO 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 ₃ CN | 1.0×10^8 *7.7 × 10 ⁷ | $(3.3 \pm 0.6) \times 10^{-4}$ | rt | Ad-15 | | Beth.77F113 |
| 9.6.4 | | CH ₃ CN | $k_{\rm r} = 1.0 \times 10^8$ *2.7 × 10 ⁷ | | rt | Ad-17 A'd | | Beth.77F113 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_{d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|--|---------------------------------|--|--|--|----------------|----------|-------------|
| | | | | COMPOUNDS | 9.7 – 9.15 : | | | |
| | | | | Q Q R ₁ -C-C-C- N | R ₂ | | | |
| | | | | R ₃ | ₹4 | | | |
| | | | | N(C21 | L) ₂ | | | |
| 9.7 | $R_1 = t - Bu$ $R_2 = t - Bu$ | C_5H_5N | $\approx 1.6 \times 10^{7}$ $\approx *3.0 \times 10^{7}$ | | rt | Od-20 | a | Smit75F1 |
| | $\mathbf{R}_3 = \mathbf{H}$ | | (est) | | | | • | |
| 9.8 | $R_4 = Et$ $R_1 = Ph$ | C ₅ H ₅ N | $\approx 1.6 \times 10^7$ | | rt | Od-20 | a | Smit75F1 |
| | $R_2 = Ph$ $R_3 = H$ | | $\approx *3.0 \times 10^{7}$ (est) | | | | | |
| 9.9 | $R_4 = Et$ $R_1 = -NHPh$ | C ₅ H ₅ N | $\approx 1.6 \times 10^7$ | | rt | Od-20 | a | Smit75F1 |
| | $R_2 = -NHPh$ $R_3 = H$ | | $\approx *3.0 \times 10^7$ (est) | | | | | |
| 9.10 ^b | $R_4 = Et R_1 = t-Bu$ | C ₅ H ₅ N | 7.9×10^{6} | | rt | Od-20 | a | Smit75F1 |
| | $R_2 = -NHPh$ $R_3 = H$ | 5 5 | *1.5 \times 10 ⁷ | | | | | |
| 9.11 ^b | $R_4 = H$ $R_1 = t-Bu$ | C₅H₅N | 2.5×10^{6} | | rt | Od-20 | a | Smit75F1 |
| | $R_2 = -NHPh$ $R_3 = H$ | - 33 | * 4.8×10^7 | | | | _ | |
| 9.12 ^b | $R_4 = Me$ $R_1 = Ph$ | C ₅ H ₅ N | 4.0×10^{6} | | rt | Od-20 | a | Smit75F1 |
| | $R_2 = -NHPh$ $R_3 = H$ | O32232 1 | *7.6 \times 10 ⁶ | | •• | 9 4 2 0 | | J |
| 9.13 ^b | $R_4 = H$ $R_1 = Ph$ | C ₅ H ₅ N | 7.9×10^{6} | | rt | Od-20 | a | Smit75F1 |
| 7.13 | $R_1 = H$ $R_2 = -NHPh$ $R_3 = H$ | C511514 | $*1.5 \times 10^7$ | | 11 | Ou-20 | a | , Sime/31 1 |
| O 14b | $R_4 = Me$ | CHN | 6.3×10^{7} | | | 04.10 | _ | Smit 75E1 |
| 9.14 ^b | $R_1 = Ph$ $R_2 = -NHPh$ | C ₅ H ₅ N | $*1.2 \times 10^8$ | | rt | Od-20 | а | Smit75F1 |
| | $R_3 = Me$ $R_4 = Me$ | a w w | | | | 0.1.00 | | C : |
| 9.15 | $R_1 = -NHPh$ $R_2 = -NHPh$ | C ₅ H ₅ N | 1.6×10^{7} *3.0 × 10 ⁷ | | rt | Od-20 | а | Smit75F1 |
| | $R_3 = H$ $R_4 = H$ | | | GOL (DOLLA INC. | 0.14 0.07 | | | |
| | | | | COMPOUNDS | 9.16 – 9.27 | : | | |
| | | | | College Part Reserved Part Res | R ₁ R ₃ R ₄ | | | |
| 9.16 | $R_1 = Me$ $R_2 = H$ $R_3 = H$ $R_4 = H$ $R_5 = H$ | CH ₃ CN | 5.0×10^7 *4.0 × 10 ⁷ | | rt | Od-20 | c | Smit75F1 |

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

| No. Si | ubstrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|--|---------------------------------|--|---------------------------------------|----------|--------|------------|------------|
| 9.17 | $R_1 = Me$ $R_2 = Me$ $R_3 = Me$ | CH ₃ CN | 5.0×10^{8} *4.0 × 10 ⁸ | | rt | Od-20 | С | Smit75F166 |
| 0.40 | $R_4 = Me$ $R_5 = H$ | | | | | | | |
| 9.18 | $R_1 = Me$ $R_2 = H$ $R_3 = H$ | C ₅ H ₅ N | 4.0×10^{7} *7.6 × 10 ⁷ | | rt | Od-20 | a | Smit75F166 |
| 9.19 | $R_4 = H$ $R_5 = Me$ $R_1 = Me$ | CH₃CN | $6.3 	imes 10^6$ | | rt | Od-20 | c | Smit75F166 |
| | $R_2 = H$ $R_3 = H$ $R_4 = Me$ | | *5.0 × 10 ⁶ | | | | | |
| 9.20 | $R_5 = Me$ $R_1 = Me$ $R_2 = Me$ $R_3 = Me$ | CH ₃ CN | 4.0×10^6 $*3.2 \times 10^6$ | | rt | Od-20 | c | Smit75F166 |
| 9.21 | $R_4 = Me$ $R_5 = Me$ $R_1 = Me$ $R_2 = H$ | CH ₃ CN | 4.0×10^{8} *3.2 × 10 ⁸ | | rt | Od-20 | c | Smit75F166 |
| | $R_2 = H$ $R_3 = H$ $R_4 = H$ $R_5 = Et$ | | 3.2 × 10 | | | | | |
| 9.21.1 | , —- | C_5H_5N | 4.0×10^{7} *7.6 × 10^{7} | | rt | Od-20 | a | Smit75F166 |
| 9.21.2 | | C_6H_6 | 1.2×10^{7} | | rt | Od-20 | e | Smit75F166 |
| 9.22 ^b | $R_1 = Me$ $R_2 = H$ $R_3 = Me$ $R_4 = H$ | C ₅ H ₅ N | 4.0×10^{7} *7.6 × 10 ⁷ | | rt | Od-20 | a . | Smit75F166 |
| 9.23 ^b | $R_5 = Et$ $R_1 = Me$ $R_2 = Me$ $R_3 = Me$ | CH ₃ CN | 4.0×10^9 *3.2 × 10 ⁹ | | rt | Od-20 | c | Smit75F166 |
| | $R_4 = H$ $R_5 = Et$ | | | | | | | |
| 9.23.1 | 3 | C ₅ H ₅ N | 6.3×10^8 *1.2 × 10 ⁹ | | rt | Od-20 | a | Smit75F166 |
| 9.23.2 | D . D | C ₆ H ₆ | 1.1×10^{9} | | rt | Od-20 | e | Smit75F166 |
| 9.24 ^b | $R_1 = t-Bu$ $R_2 = H$ $R_3 = Me$ $R_4 = H$ | CH ₃ CN | 1.3×10^9 *1.0 × 10 ⁹ | | · rt | Od-20 | c | Smit75F166 |
| 9.24.1 | $R_5 = Et$ | C ₅ H ₅ N | 1.65×10^8 | | rt | Od-20 | a | Smit75F166 |
| 9.24.2 | | C ₆ H ₆ | $^{*3.1} \times 10^{8}$ 1.3×10^{8} | | rt | Od-20 | e | Smit75F166 |
| 9.25 ^b | $R_1 = t-Bu$ $R_2 = Me$ $R_3 = Me$ $R_4 = H$ | C ₅ H ₅ N | 1.0×10^9 *1.9 × 109 | | rt | Od-20 | a | Smit75F166 |
| 9.26 | $\begin{array}{l} R_5 = Et \\ R_1 = -NHCOPh \\ R_2 = Me \\ R_3 = Me \end{array}$ | C ₅ H ₅ N | 1.0×10^9 *1.9 × 109 | | rt | Od-20 | a | Smit75F166 |
| | $R_4 = H$ $R_5 = Et$ | | | , | | | | |

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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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|---|---------------------------------|--|---------------------------------------|-----------|--------|--|------------|
| 9.27 | $R_1 = Me$ $R_2 = H$ $R_3 = H$ $R_4 = H$ | C ₅ H ₅ N | 5.0×10^{7} *9.5 × 10 ⁷ | | rt | Od-20 | a | Smit75F166 |
| 9.28 | $R_5 = Ph$ $C_6H_5 \longrightarrow N \longrightarrow N$ $O \longrightarrow N \longrightarrow CH_3$ | CH₃CN | (not measurable) | | rt | Od-20 | S = RB, $A' = 2M2P$. No measurable effect. | Smit75F166 |
| 9.28.1 | о́сн ₃ | C5H5N | (not measurable) | | rt | Od-20 | S = RB, A' = 2M2P. | Smit75F166 |
| 9.29 | C ₆ H ₅ _N—N | CH₃CN | (not measurable) | | rt | Od-20 | No measurable effect. S = RB, A' = 2M2P. No measurable effect. | Smit75F166 |
| | CH ₃ CH ₃ CH ₃ CH ₃ CH ₃ CH ₅ N O CH ₅ N O CH ₅ N O C ₆ H ₅ | | | | | | | |
| 9.29.1 | | C ₅ H ₅ N | (not measurable) | | rt | Od-20 | S = MB, A' = 2M2P. No measurable effect. | Smit75F166 |
| 9.30 ^b | | C ₅ H ₅ N | 1.0×10^9 *1.9 × 10° | | rt | Od-20 | a a | Smit75F166 |
| | CH ₃ N CH ₃ CH ₃ N(C ₂ H ₅) ₂ | | | | | | | è |
| | | | | COMPOUNDS 9. | 31 – 9.32 | | | |
| | | | | | | | | |
| 9.31 | $R_1 = H$ | C ₅ H ₅ N | $\leq 4.0 \times 10^{7}$ | | rt | Od-20 | a | Smit75F166 |
| 9.32 | $R_2 = -Ph$ $R_1 = -Ph$ $R_2 = -Ph$ | C_5H_5N | | | rt | Od-20 | a | Smit75F166 |
| 9.33 | $\mathbf{R}_2 = -\mathbf{P}\mathbf{h}$ | CH ₃ CN | 3.9×10^{10} *3.1 × 10 ¹⁰ | | rt | Od-20 | a | Smit75F166 |
| | C-NH- | SO ₂ F | | | | | | |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--|---|---|---------------------------------------|-------------|----------------|--|--------------------------|
| 9.33.1 | C ₅ H ₅ N | 1.35 × 10 ⁹ *2.6 × 10 ⁹ | | rt | Od-20 | a | Smit75F166 |
| 9.33.2 9.34 | C ₆ H ₆ MeOH | 4.7×10^9 $k_{\rm r} \approx 4.0 \times 10^5$ | | rt rt | Od-20 Ad-15 | e d | Smit75F166 Byer76F07 |
| (C ₂ H ₅ | C ₂ H ₅) 1- | *2.1 × 10 ⁵ | | | | | |
| 9.35 | МеОН | $k_{\rm r} = 4.0 \times 10^5$ $\approx *2.1 \times 10^5$ | | rt | Ad-15 | d | Byer76F07 |
| (C ₂ H ₉ | $\left(\sum_{C_2H_5}^{S}\right)\alpha^{-1}$ | | | | | | |
| 9.36 | МеОН | $k_{\rm r} = 3.4 \times 10^7$ *1.8 × 10 ⁷ | | rt | Ad~15 | d , | Byer76F07 |
| C ₂ H ₅ | C ₂ H ₅ | | | | | | |
| | | , | COMPOUNDS | 9.37 – 9.39 | : | | |
| | | | 6 7 S C2H5 | S 5 5 X - | | | |
| $9.37 X = TOS^{-}$ | МеОН | $k_{\rm r}=3.5\times10^6$ | | | A J 15 | ı | D . 7(F07) |
| $9.38 	 X = TOS^{-}$ | МеОН | $k_{\rm r} = 3.3 \times 10^{6}$ $k_{\rm r} = 6.7 \times 10^{6}$ | | rt rt | Ad-15 Ad-15 | d d | Byer76F071 Byer76F071 |
| $R_5 = R_{5'} = -6$ $9.39 	 X = Br^-$ | OMe MeOH | *3.5 \times 10 ⁶ $k_{\rm r} = 1.3 \times 10^6$ | | rt | Ad-15 | d | Byer76F071 |
| $R_5 \approx R_{5'} = -6$ 9.40 | CI MeOH | * 6.8×10^{5} $k_{\rm r} = 1.6 \times 10^{7}$ * 8.4×10^{6} | ÷ | rt | Ad-15 | d | Byer76F071 |
| S N+ C ₂ H ₅ | S TOS | × . | | | | | |
| C ₂ H ₅ -N | MeOH | $k_{\rm r} = 1.1 \times 10^8$ *5.8 × 10 ⁷ | | , rt | Ad-15 | S = 2-acetonaphthone, RB,Py, and fluorenone. k derived using $\Phi(^{1}O_{2}^{*})$ production) for each S and $k_{d} = 1.9 \times 10^{5}$ (*1.0 × 10 ⁵) s ⁻¹ [1.3.1]. k_{r} is an average for the 4 | Byer76F071 |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|--------------------|--|---------------------------------------|--|--------|---|------------|
| 9.41.1 | | CD ₃ OD | $k_r = 1.6 \times 10^8$ (est) | | rt | Ad-15 | S = 2-acetonaphthone. k estimated using $\Phi(^{1}O_{2}^{*} \text{ production}) = 0.75$ and $k_{d} = 1.3 \times 10^{4}$ s ⁻¹ (calc). | Byer76F071 |
| | | | | COMPOUNDS | 9.42 - 9.45 : | | s (caic). | |
| | | | | 6 7 S C2H3 | S 6' X - C ₂ H ₅ | | | , |
| 9.42 | $X = Br^{-}$ | МеОН | $k_{\rm r} = 1.6 \times 10^7$ *8.4 × 10 ⁶ | | rt | Ad-15 | d | Byer76F071 |
| 9.43 | $R_5 = R_{5'} = -OM6$ $X = TOS^-$ | MeOH | $k_{\rm r} = 3.1 \times 10^7$ *1.6 × 10 ⁷ | | rt | Ad-15 | d | Byer76F071 |
| 9.44 | $R_5 = R_{5'} = -Cl$ $X = Br^-$ | MeOH | $k_{\rm r} = 7.1 \times 10^6$ *3.7 × 10 ⁶ | | rt | Ad-15 | d | Byer76F071 |
| 9.45 | $R_5 = R_{5'} = -CN$ $X = BF_4^-$ | MeOH | $k_{\rm r} = 3.3 \times 10^6$ *1.7 × 10 ⁶ | | rt | Ad-15 | d | Byer76F071 |
| 9.46 | 11 - 21 4 | МеОН | $k_r = 7.3 \times 10^7$ *3.8 × 10 ⁷ | | rt | Ad-15 | d | Byer76F071 |
| | \$ | 5 V 2445 | Br [−] | | | | | |
| 9.47 | | МеОН | $k_{\rm r} = 2.9 \times 10^8$ *1.5 × 10 ⁸ | | rt | Ad-15 | d | Byer76F07 |
| | C ₂ H ₅ | Tos- | | | | | | |
| 9.48 | | МеОН | $k_{\rm r} \leqslant 3.0 \times 10^4$ *1.6 × 10 ⁴ | | rt | Ad-15 | d | Byer76F07 |
| | Ch2 CH3 | NH ONS | I- | | | | | |
| 9.49 | | МеОН | $k_{\rm r} = 1.2 \times 10^8$ *6.3 × 10 ⁷ | | rt | Ad-15 | d . | Byer76F071 |
| | C ₂ H ₅ | TOS- | | | | | | |

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

| No. | Substrate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|------|---------------------------------------|---|---|---------------------------------------|----------|--------|---|-------------|
| 9.50 | | МеОН | $k_{\rm r} = 1.5 \times 10^8$ *7.8 × 10 ⁷ | | rt | Ad-15 | d | Byer76F071 |
| | C2H3 | i- | | | | | | |
| 9.51 | | МеОН | $k_{\rm r} = 2.7 \times 10^7$ *1.4 × 10 ⁷ | | rt | Ad-15 | d | Byer76F071 |
| | |) ₁ - | | | | | | |
| 9.52 | | МеОН | $k_r = 1.3 \times 10^7$ *6.8 × 10 ⁶ | • | rt | Ad-15 | d | Byer76F071 |
| | C ₂ H ₅ | C ₂ H ₅ | | | | | | |
| 9.53 | | МеОН | $k_{\rm r} = 5.1 \times 10^7$ *2.7 × 10 ⁷ | | rt | Ad-15 | d | Byer76F071 |
| | C2H5 | $\left(\begin{array}{c} s \\ c_{2}H_{5} \end{array}\right)$ | 1- | | | | | |
| 9.54 | | CH ₃ CN | $(3.0 \pm 0.8) \times 10^{10}$ | | rt | A'd-5 | S = MB, A' = DPBF, ruby laser (694 nm). | Merk.72F260 |
| | C ₆ H ₅ CH=CH=C | CH=CH-CH | 5) CIO- | | | | | |

^aS = RB, A' = 2-methyl-2-pentene. k derived using $\beta_{A'} = 4.3 \times 10^{-2}$ mol dm⁻³ [2.40.19] $k_{\rm d} = 3.1 \times 10^4$ (*5.9 × 10⁴) s⁻¹ [1.29]. No evidence of chemical reaction.

°S = RB, A' = 2-methyl-2-pentene.
$$k$$
 derived using $\beta_{A'} = 1.8 \times 10^{-2}$ mol dm⁻³ [2.40.11] and $k_{\rm d} = 3.3 \times 10^4$ (*2.6 × 10⁴) s⁻¹ [1.17]. No evidence of chemical reaction.

^dS = 2-acetonaphthone. k derived using
$$Φ(^1O_2* \text{ production}) = 0.75$$
 and $k_d = 1.9 \times 10^5$ (*1.0 × 10⁵) s⁻¹ [1.3.1].

^eS = azine, A' = 2-methyl-2-pentene.
$$k$$
 derived using $\beta_{A'} = 5.3 \times 10^{-2}$ mol dm⁻³ [2.40.23] and $k_{\rm d} = 4.2 \times 10^4$ s⁻¹ [1.32]. 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.

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

| No. | Substrate (Q) | Solvent / | $k_{\rm q}$ dm ³ mol ⁻¹ s ⁻¹ | t /°C | Method | Comments | Ref. |
|---------|--|--------------------------------------|---|----------|--------|--|--------------|
| 10.1 | NiCl ₂ -6H ₂ O | 2-butoxy- ethanol | 3.1 × 10 ⁸ (est) | 0 | Ad-33 | $^{1}O_{2}$ * from microwave discharge, A = Rub. k estimated using k_{d} = 3.8×10^{5} s ⁻¹ [$I(a)$.4] and k_{A} = 7×10^{7} dm ³ mol ⁻¹ s ⁻¹ . | Carl72F31 |
| 10.2 | CoCl ₂ ·6H ₂ O | 2-butoxy- ethanol | 4.8×10^7 (est) | 0 | Ad-33 | $^{1}\text{O}_{2}^{*}$ from microwave discharge, $A = \text{Rub. } k \text{ estimated using } k_{\text{d}} = 3.8 \times 10^{5} \text{ s}^{-1} [1(a).4] \text{ and } k_{\text{A}} = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}.$ | Carl72F31 |
| 10.3 | MnCl ₂ ·6H ₂ O | 2-butoxy- ethanol | $ < 1.0 \times 10^6 $ (est) | 0 | Ad-33 | $^{1}O_{2}$ * from microwave discharge, A = Rub. k estimated using k_{d} = 3.8 × 10 ⁵ s ⁻¹ [$I(a)$.4] and k_{A} = 7×10^{7} dm ³ mol ⁻¹ s ⁻¹ . | Carl72F31 |
| 10.4 | MnCl ₂ ·4H ₂ O | i-octane | $\leq 1.0 \times 10^6$ (est) | 25 | Ad-23 | | Carl74F341 |
| 10.5 | Ni(II) bis[hydrotris- (1-pyrazoyl)- borate] | CHCl ₃ | $(2.1 \pm 0.4) \times 10^6$ | rt | Ad-33 | | Monr.79A05 |
| | $HB\left(\left\langle \bigcirc_{N-N}\right\rangle \right)_3\equiv L$ | | | | | | |
| 10.6 | Ni(II) bis[isopropyl-xanthate] | i-octane | 5.4×10^9 (est) | 25 | Ad-23 | S = A = Rub. k estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Carl.74F642 |
| 10.7 | [(CH ₃) ₂ CHOCS ₂] ₋₂ Ni Ni(II) bis(N-phenyl- dithiocarbamate) [C ₄ H ₄ NHCS ₂] ₂ Ni | CHCl ₃ | $(1.1 \pm 0.2) \times 10^{10}$ | rt | Ad-33 | and $k_d = 4.0 \times 10^4 \text{ s}^{-1}[I(a).6]$ $S = A = \text{Rub. } k \text{ derived using } k_A = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [3.63.3]$ and $k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5]$. | Monr.79A05 |
| 10.8 | Ni(II) bis(N,N -dimethyl-dithiocarbamate) { $(CH_3)_2NCS_3$ }Ni | CH ₂ Cl ₂ | 1.8×10^7 | rt | A'd-19 | S = A = Tetr. k derived using $k_A = 3.0 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. [3.62]. | Byst.75F654 |
| 10.8.1 | ((3.23,7,2.1.3.2,1,2.1.1. | | not measurable | 22 | Pa-13 | S = RB, A = TMHP, P = nitroxy | Ivan75F44 |
| 10.9 | Ni(II) bis(N,N-diethyl-dithiocarbamate) [(CH ₃ CH ₂) ₂ ,NCS ₂] ₂ Ni | (8:1) v:v CCl₄/MeOH (98:2) v:v | $(6.6 \pm 0.6) \times 10^9$ | rt | Ad-5 | radicals. $S = MB$, $A = DPBF$, flash photolysis. | Furu.78E238 |
| | | | LIGANDS 10.10 - | 10.15 : | | | |
| | | | CH ₃ S (CH ₃ CH) ₂ NC S | ≣L | | | |
| 10.10 | Mn(II) bis(N,N-diiso-propyldithiocarbamate) | CH ₂ Cl ₂ | $< 1.0 \times 10^7$ (est) | rt | Ad-23 | S = A = Rub. k estimated using $k_A = 7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 7.3 \times 10^3 \text{ s}^{-1}$. | Carl73P066 |
| 10.11 | Co(II) bis(N,N-diiso-propyldithiocarbamate) | CH ₂ Cl ₂ | 1.9×10^9 (est) | rt | Ad-23 | | Carl73P066 |
| 10.11.1 | | i-octane | 1.9×10^{9} | 25 | Ad-23 | | Carl74F341 |
| 10.11.2 | | hexadecane | (est) 9.0 × 10 ⁸ (est) | 25 | Ad-33 | $k_A = 7.3 \times 10$ dm mol s. ${}^{1}O_2$ * from a microwave discharge, A = Rub. k estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ and}$ $k_d = 9.0 \times 10^4 \text{ s}^{-1} [I(a). 7].$ | Carl.,74F341 |
| 10.12 | Ni(II) bis(N,N-diiso- propyldithiocarbamate) | CH ₂ Cl ₂ | 3.4×10^{9} (est) | rt | Ad-23 | $S = A = Rub. k$ estimated using $k_A = 7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 7.3 \times 10^3 \text{ s}^{-1}$. | Carl73P066 |
| 10.13 | Cu(II)bis(N,N-diiso-propyldithiocarbamate) | CH ₂ Cl ₂ | $< 1.0 \times 10^7$ (est) | rt | Ad-23 | $k_{\rm d} = 7.3 \times 10^{3} \text{k}$ estimated using $k_{\rm A} = 7.3 \times 10^{7} \text{dm}^{3} \text{mol}^{-1} \text{s}^{-1}$ and $k_{\rm d} = 7.3 \times 10^{3} \text{s}^{-1}$. | Carl73P066 |

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

| No. | Substrate (Q) | Solvent /c | $\frac{k_{\rm q}}{{ m dm}^3~{ m mol}^{-1}~{ m s}^{-1}$ | t /°C | Method | Comments | Ref. |
|--------|--|---|--|---------------|--------|--|------------|
| 0.14 | Zn(II) bis(N,N-diiso- propyldithiocarbamate) | CH ₂ Cl ₂ | $ < 1.0 \times 10^7 $ (est) | rt | Ad-23 | S = A = Rub. k estimated using $k_A = 7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 7.3 \times 10^3 \text{ s}^{-1}$. | Carl73P06 |
| 0.15 | Fe(III) bis(N,N-diiso- propyldithiocarbamate) | CH ₂ Cl ₂ | 3.8×10^9 (est) | rt | Ad-23 | = | Carl73P06 |
| 0.15,1 | 1 | CH ₂ Cl ₂ | 4.3×10^9 (est) | 25 | Ad-23 | | Carl74F34 |
| 0.15.2 | | CH ₂ Cl ₂ | 3.9×10^9 (est) | 25 | Ad-23 | | Carl.74F64 |
| 0.15.3 | | i-octane | 3.8×10^9 (est) | 25 | Ad-23 | $K_d = 7.3 \times 10^{-3} \text{ s}$ S = A = Rub. k estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ and}$ $k_d = 4.0 \times 10^4 \text{ s}^{-1} \{I(a).6\}.$ | Carl.74F64 |
| 0.15.4 | | hexadecane | 1.2×10^9 (est) | 25 | Ad-33 | 1 O 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]. | Carl74F34 |
| | | | LIGANDS 10.16 | - 10.19 : | | ing soo / to o [x(a), / j. | |
| | | | (CH3CH2CH2CH2)2NC | S ≊L ;⊖ | | | |
| 0.16 | 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.78E23 |
| 0.17 | Ni(II) bis(N,N-dibutyl-dithiocarbamate) | CH ₂ Cl ₂ | 9.0×10^9 (est) | 25 | Ad-23 | S = A = Rub. k estimated using $k_A = 7.3 \times 10^7 \text{dm}^3 \text{mol}^{-1} \text{s}^{-1}$ and $k_d = 8 \times 10^3 \text{s}^{-1}$. | Carl74F34 |
| 0.17.1 | | CH ₂ Cl ₂ | 8.0×10^{9} (est) | 25 | Ad-23 | $K_d = 3 \times 10^{-3} \text{ s}$. S = A = Rub. k estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ and}$ $k_d = 7.3 \times 10^3 \text{ s}^{-1}$. | Carl.74F64 |
| 0.17.2 | | CH ₂ Cl ₂ | 5.7×10^9 | rt | A'd-19 | S = A = Tetr. k derived using $k_A = 3.0 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. [3.62]. | Byst.75F65 |
| 0.17.3 | | CHCl ₃ | $(8.1 \pm 1.3) \times 10^9$ | rt | Ad-33 | • • | Monr.79A0 |
| 0.17.4 | | C₀H₅Br | 2.6×10^8 (est) | 0 | Ad-33 | | Guil.73F33 |
| 0.17.5 | | C ₆ H ₅ CH ₃ | 4.3×10^9 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P0 |
| 0.17.6 | | i-octane | 7.0×10^9 (est) | 25 | Ad-23 | $K_A = 1.7 \times 10^{4} \text{ dm}^{2} \text{ min}^{2} \text{ s}^{-1}$ S = A = Rub. k estimated using $k_A = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 4.0 \times 10^{4} \text{ s}^{-1} [1(a).6]$. | Carl72F3 |
| 0.17.7 | | i-octane | 1.7×10^{10} (est) | 25 | Ad-23 | S = A = Rub. k estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 4.7 \times 10^4 \text{ s}^{-1}$ [I(a).6.1]. | Carl74F34 |
| 0.17.8 | | hexadecane | 1.0 × 10 ⁹ (est) | 25 | Ad-33 | and $k_d = 4.7 \times 10^{-5}$ [14).6.1]. ${}^{1}O_{2}^{*}$ from a microwave discharge, $A = \text{Rub. } k \text{ estimated using } k_A = 7.3 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1} \text{ and}$ $k_d = 9.0 \times 10^{4} \text{ s}^{-1} [1(a).7].$ | Carl74F34 |
| 0.17.9 | | hexadecane | 9.0×10^8 (est) | 25 | Ad-33 | $^{1}\text{O}_{2}$ * from a microwave discharge, A = Rub. k estimated using $k_{A} = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{d} = 9.0 \times 10^{4} \text{ s}^{-1} [I(a).7]$. | Carl72F3 |

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

| No. | Substrate (Q) | Solvent | $k_{\rm q}$ $/{ m dm}^3~{ m mol}^{-1}~{ m s}^{-1}$ | <i>t</i> /°C | Method | Comments | Ref. |
|---------|---|--|--|-----------------|--------|---|-------------|
| 10.17.1 | 0 | CCl ₄ /MeOI (98:2) v:v | $H (4.1 \pm 0.6) \times 10^9$ | rt | Ad-5 | S = MB, A = DPBF, flash photolysis. | Furu.78E23 |
| 10.17.1 | 1 | ` , | $(4.0 \pm 1.5) \times 10^9$ | rt | Ad-5 | S = MB, $A = DPBF$, flash photolysis. | Floo73F33 |
| 10.17.1 | 2 | C ₆ H ₆ /EtOH (8:1) v:v | $\begin{array}{c} 1.6 \times 10^9 \\ \text{(est)} \end{array}$ | 22 | Pa-13 | S = RB, A = TMHP, P = Nitroxy radicals. k estimated using $k_d = 3 \times 10^4 \text{s}^{-1}$ (calc). | Ivan75F4 |
| 10.17.1 | | CH ₂ Cl ₂ /Me /C ₅ H ₅ N (94:3:3) v:v: | OH < 1.0 × 10 ⁹ (est) | 25 | Ad-32 | $^{1}O_{2}*$ from (PhO) ₃ PO ₃ decomp., 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 . Interference by chelate ozonide reaction to give colored products. | Carl72F31 |
| 10.18 | Cu(II) bis(N,N-dibutyl-dithiocarbamate) | CCl₄/MeOI (98:2) v:v | $I < 5 \times 10^8$ | rt | Ad-5 | S = MB, $A = DPBF$, flash photolysis. | Furu.78E238 |
| 10.19 | Zn(II)bis(N,N-dibutyl-dithiocarbamate) | ` ' | $(2.0 \pm 1.0) \times 10^7$ | rt | Ad-5 | S = MB, $A = DPBF$, flash photolysis. | Floo73F33 |
| 10.19.1 | · | C ₆ H ₅ Br | $\leqslant 1 \times 10^6$ (est) | 0 | Ad-33 | ¹ O ₂ * from microwave discharge, A' = Rub. No measurable effect. | Guil.73F333 |
| 10.20 | Ni(II)bis(N,N-di- phenyldithiocarbamate) [(C ₆ H ₅) ₂ NCS ₂] ₂ Ni | CHCl ₃ | $(6.3 \pm 1.0) \times 10^9$ | rt | Ad-33 | $S = A = Rub. k$ derived using $k_A = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [3.63.3]$ and $k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5]$. | Monr.79A05 |
| 10.20.1 | | i-octane | $< 1.0 \times 10^6$ (est) | 25 | Ad-23 | $S = A = Rub. k$ estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 4.7 \times 10^4 \text{ s}^{-1} [I(a).6.1]$. | Carl74F341 |
| 10.21 | Ni(II) bis[N-(p-methyl phenyl)dithiocarbamate] [(4-CH ₃ C ₆ H ₄)NHCS ₂] ₂ Ni | CHCl ₃ | $(1.1 \pm 0.2) \times 10^{10}$ | rt | Ad-33 | _ | Monr.79A050 |
| 10.22 | Ni(II) bis[O-ethyl-3,5-di-t-butyl-4-hydroxy-benzylphosphonate] | CH ₂ Cl ₂ | 6.0×10^{6} | rt | A'd-19 | S = A = Tetr. k derived using $k_A = 3.0 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.62]. | Byst.75F654 |
| 10.22.1 | (CH ₃) ₃ C | CHCl ₃ | $(2.2 \pm 0.4) \times 10^7$ | rt | Ad-33 | S = A = Rub. k derived using k_A = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [3.63.3]$ and k_d = $1.67 \times 10^4 \text{ s}^{-1} [1.5]$. | Monr.79A05 |
| 10.23 | Ni(II) bis[O-butyl- 3,5-di-t-butyl- 4-hydroxybenzyl- phosphonate] | CH ₂ Cl ₂ | 1.4×10^7 (est) | 25 | Ad-23 | S = A = Rub. k estimated using $k_A = 7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 7.3 \times 10^3 \text{ s}^{-1}$. | Carl72F319 |
| 10.23.1 | OH C(CH ₃) ₃ CH ₃ (CH ₂) ₂ CH ₂ O P O O | CH ₂ Cl ₂ | 1.6×10^{7} (est) | 25 | Ad-23 | S = A = Rub. k estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 7.3 \times 10^3 \text{ s}^{-1}$. | Carl.74F642 |
| 0.23.2 | | 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 | $^{1}\text{O}_{2}$ from microwave discharge, $A = \text{Rub. } k \text{ estimated using } k_{d} = 3.8 \times 10^{5} \text{ s}^{-1} [1(a).4] \text{ and } k_{A} = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}.$ | Carl72F319 |
| 0.23.4 | | C₄H₃Br | 1.3 × 10 ⁷ (est) | 0 | Ad-33 | $^{1}O_{2}$ * from microwave discharge, $A = \text{Rub. Measured } k/[(k_{d}/[A]) + k_{A}] = 0.1 \text{ at } [A] = 1.5 \times 10^{-4} \text{ mol dm}^{-3} \cdot k \text{ estimated using } k_{A} = 4.0 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1} \text{ and } k_{d} = 1.3 \times 10^{4} \text{ s}^{-1} [1.34].$ 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 ₆ H ₅ CH ₃ | 2.0 × 10 ⁸ (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_d = 1.7 \times 10^8 \text{ dm}^3 \text{ mal}^{-1} \text{ s}^{-1}$ | Zwei.75P063 |
| 10.23.6 | | CCl ₄ /CHCl (9:1) v:v | $1_3 9.0 \times 10^6$ | rt | Ad-23 | $k_{\rm A} = 1.7 \times 10^8 {\rm dm^3 \ mol^{-1} \ s^{-1}}.$ $S = A = {\rm Rub. \ Measured}$ $k_{\rm Q}/(k_{\rm A} A] + k_{\rm d}) = 5.2 \times 10^3 {\rm dm^3 \ mol^{-1} \ at \ \{A\}} = 5 \times 10^{-6} {\rm mol \ dm^{-3}}. \ k_{\rm Q} {\rm derived \ using} \ k_{\rm A} = 7 \times 10^7 {\rm dm^3 \ mol^{-1} \ s^{-1} \ and} \ k_{\rm d} = 1.43 \times 10^3 {\rm s^{-1}} [1.8].$ | Hrdl74F64 |
| 10.23.7 | | CH ₂ Cl ₂ /M ₆ /C ₅ H ₅ N (94:3:3) v:v | eOH 1.0 × 10 ⁷ (est) | 25 | Ad-32 | $^{1}O_{2}^{*}$ from $(PhO)_{3}PO_{3}$ decomp., A = Rub. k estimated using k_{A} = 7×10^{7} dm ³ mol ⁻¹ s ⁻¹ and $k_{d} = 7.3 \times 10^{3}$ s ⁻¹ . | Carl72F31 |
| | | | LIGANDS 10.24 A | ND 10 | 0.26 : | | |
| | | | RO P S | =L | | | · . |
| 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 = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [3.63.3]$ and $k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5]$. | Monr.79A05 |
| 10.25 | Ni(II) bis[O,O'-diiso- propyldithio- phosphate] [R = -i-Pr] | CH ₂ Cl ₂ | 5.4×10^9 (est) | rt | Ad-23 | | Carl73P066 |
| 10.25.1 | | CCl ₄ /MeOl (98:2) v:v | H $(7.6 \pm 1.0) \times 10^9$ | rt | Ad-5 | S = MB, A = DPBF, flash photolysis. | Furu.78E238 |
| 10.26 | Co(II) bis[O , O' -dicyclo-hexyldithio-phosphate] [$R = -cyclo - C_e H_{11}$] | C ₆ H ₅ CH ₃ | $\begin{array}{c} 2.7 \times 10^9 \\ \text{(est)} \end{array}$ | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| 10.27 | Ni(II) bis(dicyclo- hexyldithio- phosphinate) [(cyclo-C ₆ H ₁₁) ₂ PS ₂] ₂ Ni | CHCl ₃ | $(5.7 \pm 0.9) \times 10^9$ | rt | Ad-33 | S = A = Rub. k derived using $k_A = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \{3.63.3\}$ and $k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5]$. | Monr.79A05 |
| | 107011 061-11722 02122 12 | | LIGANDS 10.28 - | 10.33 | | | |
| | | | C ₆ H ₅ O P S | •L | | • | |
| 10.28 | Co(II) bis(O,O'-di- phenyldithiophosphate) | C_6H_6 | 1.2×10^{9} | rt | Ad-23 | $S = A = Rub. k derived using k_A = 3 \times 10^7 dm^3 mol^{-1} s^{-1} and k_d = 2.8 \times 10^4 s^{-1}.$ | Edil78F49 |
| 10.29 | Ni(II) bis(O,O'-di- phenyldithiophosphate) | CHCI ₃ | $(1.1 \pm 0.2) \times 10^{10}$ | rt | Ad-33 | $S = A = Rub. k derived using k_A = 5.3 \times 10^7 dm^3 mol^{-1} s^{-1} [3.63.3]$ | Monr.79A05 |
| 10.29.1 | | C ₆ H ₆ | 2.5 × 10° | rt | Ad-23 | and $k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5]$. S = A = Rub. k derived using $k_A = 3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 2.8 \times 10^4 \text{ s}^{-1}$. | Edil78F49 |
| 10.30 | Cu(II) bis(O,O'-di- phenyldithiophosphate) | C ₆ H ₆ | 1.7×10^{6} | rt | Ad-23 | and $k_d = 2.8 \times 10^{7} \text{ s}^{-1}$. $S = A = \text{Rub. } k \text{ derived using } k_A = 3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 2.8 \times 10^4 \text{ s}^{-1}$. | Edil78F49 |
| 10.31 | Zn(II) bis(O,O'-di- phenyldithiophosphate) | C ₆ H ₆ | 5.0×10^6 | rt | Ad-23 | S = A = Rub. k derived using $k_A = 3 \times 10^7 dm^3 mol^{-1} s^{-1}$ | Edil78F49 |
| 10.32 | Cr(II) bis(O,O'-di- phenyldithiophosphate) | C_6H_6 | 3.2×10^6 | rt | Ad-23 | and $k_d = 2.8 \times 10^4 \text{ s}^{-1}$. S = A = Rub. k derived using $k_A = 3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 2.8 \times 10^4 \text{ s}^{-1}$. | Edil78F49 |

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

| No. | Substrate (Q) | Solvent | $k_{\rm q}$ /dm ³ mol ⁻¹ s ⁻¹ | t /°C | Method | Comments | Ref. |
|-------|---|-------------------------------|--|--------------------------|--------|---|-----------|
| 10.33 | Pb(II) bis(O,O'-di- phenyldithiophosphate) | C ₆ H ₆ | 3.4×10^7 | rt | Ad-23 | $S = A = Rub. k derived using k_A = 3 \times 10^7 dm^3 mol^{-1} s^{-1} and k_d = 2.8 \times 10^4 s^{-1}.$ | Edil78F49 |
| | | | LIGANDS 10.34 | 1 – 10.36 : | | and $k_d = 2.0 \text{ A/10 S}$. | |
| | | | (CH ₅) ₃ C | S =1 | _ | | |
| | | | (CH3)3C | ~ S⊖ | | | |
| 10.34 | Co(II) bis(O,O'-di- p-t-butylphenyldithio- phosphate) | C ₆ H ₆ | 1.2×10^9 | rt | Ad-23 | $S = A = Rub$. k derived using $k_A = 3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 2.8 \times 10^4 \text{ s}^{-1}$. | Edil78F49 |
| 10.35 | Ni(II) bis(O,O'-di- p-t-butylphenyldithio- phosphate) | C ₆ H ₆ | 2.3×10^9 | rt | Ad-23 | S = A = Rub. k derived using $k_A = 3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 2.8 \times 10^4 \text{ s}^{-1}$. | Edil78F49 |
| 10.36 | Cu(II) bis(O,O'-di- p-t-butylphenyldithio- phosphate) | C ₆ H 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 $k_d = 2.8 \times 10^4 s^{-1}$. | Edil78F49 |
| | | | LIGANDS 10.37 | 7 – 10.39 : | | u | |
| | | | H ₉ C O | ∕s 's ^Θ •∟ | | | |
| 10.37 | Co(II) bis(O,O'-di- | C_6H_6 | 1.1 × 10° | rt | Ad-23 | | Edil78F49 |
| 10.38 | 4-methylphenyldithio- phosphate) Ni(II) bis(O,O'-di- | C_6H_6 | 2.3 × 10° | rt | Ad-23 | | Edil78F49 |
| 10.39 | 4-methylphenyldithio- phosphate) Cu(II) bis(O,O'-di- 4-methylphenyldithio- | C_6H_6 | 2.0×10^6 | rt | Ad-23 | $k_{\rm A} = 3 \times 10^7 {\rm dm^3 \ mol^{-1} \ s^{-1}}$ and $k_{\rm d} = 2.8 \times 10^4 {\rm s^{-1}}$. $S = A = {\rm Rub.} \ k \ {\rm derived \ using}$ $k_{\rm A} = 3 \times 10^7 {\rm dm^3 \ mol^{-1} \ s^{-1}}$ | Edil78F49 |
| | phosphate) | | LIGANDS 10.40 | 0 –10.44 : | | and $k_{\rm d} = 2.8 \times 10^4 {\rm s}^{-1}$. | |
| | | | (CH ₃) ₃ C | > _P | L | | |
| 10.40 | Co(II) bis[2,2'-thiobis- (O,O'-di-p-t-butylphenyl)- | C ₆ H ₆ | 8.7×10^8 | rt | Ad-23 | S = A = Rub. k derived using $k_A = 3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ | Edil78F49 |
| 10.41 | dithiophosphate] Ni(II) bis[2,2'-thiobis- (O,O'-di-p-t-butylphenyl)- dithiophosphate] | C_6H_6 | 2.2×10^9 | rt | Ad-23 | $k_{\rm A} = 3 \times 10^7 \rm dm^3 mol^{-1} s^{-1}$ | Edil78F49 |
| 10.42 | dithiophosphate] Zn(II) bis[2,2'-thiobis- (O,O'-di-p-t-butylphenyl)- dithiophosphate] | C ₆ H ₆ | 4.35×10^{6} | rt | Ad-23 | and $k_d = 2.8 \times 10^4 \text{s}^{-1}$. S = A = Rub. k derived using $k_A = 3 \times 10^7 \text{dm}^3 \text{mol}^{-1} \text{s}^{-1}$ and $k_d = 2.8 \times 10^4 \text{s}^{-1}$. | Edil78F49 |

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

| No. | Substrate (Q) | Solvent / | $k_{\rm q}$ $dm^3 mol^{-1} s^{-1}$ | t /°C | Method | Comments | Ref. |
|---------|--|---|--------------------------------------|----------------|--------|--|-------------|
| 10.43 | Cd(II) bis[2,2'-thiobis- (O,O'-di-p-t-butylphenyl)- dithiophosphate] | C ₆ H ₆ | 8.4 × 10 ⁶ | rt | Ad-23 | S = A = Rub. k derived using $k_A = 3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ | Edil78F49 |
| 10.44 | Pb(II) bis[2,2'-thiobis- (O,O'-di-p-t-butylphenyl)- dithiophosphate] | C ₆ H ₆ | 1.0×10^7 | rt | Ad-23 | and $k_d = 2.8 \times 10^4 \text{ s}^{-1}$. S = A = Rub. k derived using $k_A = 3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 2.8 \times 10^4 \text{ s}^{-1}$. | Edil78F49 |
| 10.45 | tris(2,2'-bipyridine) Ru(II)·Cl ₂ | CCl ₄ /MeOH (98:2) v:v | $I \leqslant 1.0 \times 10^9$ | rt | Ad-5 | S = MB, A = DPBF, flash photolysis. | Furu.78E238 |
| | - L | | | <i>′</i> . | | | |
| | | | LIGANDS 10.46 | - 10.47 | ! | | |
| | | | R NO | ≅L | , | | |
| 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 = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [3.63.3]$ and k_d = $1.67 \times 10^4 \text{ s}^{-1} [1.5]$. | Monr.79A05 |
| 10.47 | Ni(II) bis[1-(4'-methyl- phenyl)amino-2-(4'- methylphenyl)imino- cycloheptatriene] | CHCl ₃ | $(5.6 \pm 0.9) \times 10^9$ | rt | Ad-33 | S = A = Rub. k derived using k_A = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [3.63.3]$ and $k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5]$. | Monr.79A05 |
| | $[R = -4' - CH_3C_6H_4]$ | | LIGANDS 10.48 | AND 10 | 0.50 : | | |
| | | | R C S | ⊖ ■L ∋ | | | |
| 10.48 | Ni(II) bis[dithio- biacetyl] [R = -Me] | C ₆ H ₅ CH ₃ | 2.8×10^{10} (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{dm}^3 \text{mol}^{-1} \text{s}^{-1}$. | 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 | $S = A = Rub. k derived using k_A = 5.3 \times 10^7 dm^3 mol^{-1} s^{-1} [3.63.3]$ | Monr.79A050 |
| 10.50 | Ni(II) bis(dithio- benzil) | CHCl ₃ | $(1.1 \pm 0.2) \times 10^{10}$ | rt | Ad-33 | and $k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5]$. $S = A = \text{Rub. } k \text{ derived using } k_A = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [3.63.3]$ | Monr.79A050 |
| 10.50.1 | [R = -Ph] | C ₆ H ₅ CH ₃ | 2.2×10^{10} (est) | rt | Ad-25 | $k_{\rm d} = 1 \times 10^5 {\rm s}^{-1} ({\rm calc}) {\rm and}$ | Zwei.75P063 |
| | | | LIGANDS 10.51 | AND 10 | 0.52 : | $k_{\rm A} = 1.7 \times 10^8 \rm dm^3 mol^{-1} s^{-1}.$ | |
| | | | H ₃ C | s⊝ •L s⊝ | | | |
| 10.51 | Co(II) bis[μ -toluene-3,4-dithiolato]TBA ₂ | C ₆ H ₅ CH ₃ | 3.5 × 10 ⁹ (est) | rt | Ad-25 | $S = A = Rub$. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |

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

| No. | Substrate (Q) | Solvent / | $k_{\rm q}$ ${ m dm}^3~{ m mol}^{-1}~{ m s}^{-1}$ | t /°C | Method | Comments | Ref. |
|---------|--|--|---|-----------|--------|--|-------------|
| 10.52 | Ni(II) bis[μ-toluene- 3,4-dithiolato]TBA ₂ | C ₆ H ₅ CH ₃ | 5.8×10^{9} (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06. |
| 10.53 | Ni(II) bis[4-imino- 2-pentene-2-ol] H ₃ C C-0° EL | C ₆ H ₅ CH ₃ | 7.2×10^{9} (est) | rt | Ad-25 | $K_A = 1.7 \times 10^{\circ}$ dm mor s. S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1} \text{ (calc) and}$ $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06: |
| | с <u>—</u> мн | | | | | | |
| | | | LIGANDS 10.54 | - 10.62 : | | | |
| | | | CH CHOC |) | | | |
| 10.54 | Co(II) bis(acetyl-acetonate) | C ₆ H ₅ CH ₃ | 1×10^8 (est) | rt | Ad-25 | $S = A = Rub$. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| 10.54.1 | | CCl ₄ /CHCl ₃ (9:1) v:v | 1.46 × 10 ⁸ | rt | Ad-23 | S = A = Rub. Measured $k_{\rm Q}/(k_{\rm A}[{\rm A}] + k_{\rm d}) = 8.2 \times 10^4$ dm³ mol ⁻¹ at [A] = 5 × 10 ⁻⁶ mol dm ⁻³ . $k_{\rm Q}$ derived using $k_{\rm A} = 7 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ | Hrdl74F64 |
| 10.55 | Ni(II) bis(acetyl-acetonate) | CH ₂ Cl ₂ | 1.5×10^8 (est) | 25 | Ad-23 | using $k_{\rm A} = 7.3 \times 10^7 \rm dm^3 mol^{-1} s^{-1}$ | Carl74F341 |
| 10.55.1 | | CH ₂ Cl ₂ | 7.5×10^{7} (est) | rt | Ad-23 | and $k_d = 8 \times 10^3 \text{ s}^{-1}$. S = A = Rub. k estimated using $k_A = 7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 7.3 \times 10^3 \text{ s}^{-1}$. | Carl73P066 |
| 0.55.2 | | 2-butoxy- ethanol | 7.5×10^{7} (est) | 0 | Ad-33 | and $k_d = 7.3 \times 10^{-5}$ s. $^{1}O_2$ * from microwave discharge, $A = \text{Rub. } k \text{ estimated using}$ $k_d = 3.8 \times 10^{5} \text{ s}^{-1} [I(a).4] \text{ and}$ $k_A = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$. | Carl72F319 |
| 10.55.3 | | C ₆ H ₅ Br | 6.5×10^7 (est) | 0 | Ad-33 | $^{1}O_{2}^{*}$ from microwave discharge, $A = \text{Rub. Measured } k/[(k_{d}/[A]) + k_{A}] = 0.5 \text{ at } [A] = 1.5 \times 10^{-4}$ mol dm ⁻³ . k estimated using $k_{A} = 4.0 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1} \text{ and } k_{d} = 1.3 \times 10^{4} \text{ s}^{-1} [1.34].$ | Guil.73F333 |
| 10.55.4 | | C ₆ H ₅ CH ₃ | 3×10^{8} (est) | rt | Ad-25 | Q exists as a trimer in solution. $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_d = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ | Zwei.75P063 |
| 10.55.5 | | CCl ₄ /CHCl ₃ (9:1) v:v | 8.2×10^7 | rt | Ad-23 | $k_{\rm A} = 1.7 \times 10^8 {\rm dm^3 mol^{-1} s^{-1}}.$ $S = A = {\rm Rub. Measured}$ $k_{\rm Q}/(k_{\rm A}[{\rm A}] + k_{\rm d}) = 4.6 \times 10^4 {\rm dm^3 mol^{-1} at [{\rm A}]} = 5 \times 10^{-6} {\rm mol} {\rm dm^{-3}}. k_{\rm Q} {\rm derived using} k_{\rm A} = 7 \times 10^7 {\rm dm^3 mol^{-1} s^{-1} and} k_{\rm d} = 1.43 \times 10^3 {\rm s^{-1}} [1.8].$ | Hrdl74F64 |
| 10.56 | Cu(II) bis(acetyl-acetonate) | C ₆ H ₅ CH ₃ | 1×10^8 (est) | rt | Ad-25 | $k_d = 1.43 \times 10^{8} \text{ s}^{-1} [1.8].$ S = A = Rub. k estimated using $k_d = 1 \times 10^{5} \text{ s}^{-1} \text{ (calc) and}$ $k_A = 1.7 \times 10^{8} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}.$ | Zwei.75P063 |

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

| No. | Substrate (Q) | Solvent / | $k_{\rm q}$ 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 $k_Q/(k_A[A] + k_d) = 2.1 \times 10^3$ dm³ mol ⁻¹ at $[A] = 5 \times 10^{-6}$ mol dm ⁻³ . k_Q derived using $k_A = 7 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ and $k_d = 1.43 \times 10^3$ s ⁻¹ [1.8]. | Hrdl74F64 |
| 10.57 | Zn(II) bis(acetyl-acetonate) | CCl ₄ /CHCl ₃ (9:1) v:v | 1.08×10^{7} | rt | Ad-23 | $k_d = 1.43 \times 10^{-8} \text{ s} \text{ [1.8]}.$ S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 6.1 \times 10^3$ $dm^3 \text{ mol}^{-1} \text{ at } [A] = 5 \times 10^{-6}$ $mol \ dm^{-3}. k_Q \ derived \ using$ $k_A = 7 \times 10^7 \ dm^3 \ mol^{-1} \ s^{-1} \ and$ $k_d = 1.43 \times 10^3 \ s^{-1} \ [1.8].$ | Hrdl74F64 |
| 10.58 | Cr(III) tris(acetyl- acetonate) | CCl ₄ /CHCl ₃ (9:1) v:v | 5.0×10^5 | rt | Ad-23 | | Hrdl74F64 |
| 10.59 | Mn(III) tris(acetyl-acetonate) | C ₆ H ₅ CH ₃ | 5×10^8 (est) | rt | Ad-25 | | Zwei.75P063 |
| 10.60 | Fe(III) tris(acetyl-acetonate) | CCI ₄ /CHCI ₃ (9:1) v:v | 8.7 × 10 ⁷ | rt | Ad-23 | | Hrdl74F64 |
| 10.61 | Co(III) tris(acetyl-acetonate) | CCl ₄ /CHCl ₃ (9:1) v:v | 9.2×10^8 | rt | Ad-23 | | Hrdl74F64 |
| 10.62 | Ni(II) bis(acetyl- acetonate)-2H ₂ O | 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] | C₀H₅CH₃ | 3.9 × 10 ⁹ (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{dm}^3 \text{mol}^{-1} \text{s}^{-1}$. | Zwei.75P063 |
| | H ₃ C =0 ≡L | | | | | | |
| 10.64 | Ni(II) bis[dithio-acetylacetonate] | C₀H₃Br | 2.3×10^8 | 0 | Ad-23 | $^{1}O_{2}*$ 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 | $k_{\rm q}$ /dm ³ mol ⁻¹ s ⁻¹ | t /°C | Method | Comments | Ref. |
|---------|---|---|--|---------------|--------|---|-------------|
| 10.65 | Ni(II) bis(salicyl- aldehyde)-2H ₂ O | 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.79A05 |
| 10.66 | Ni(II) bis(5-bromosalicylaldehyde)· $2H_2O$ [$R_5 = -Br$] | CHCl ₃ | $(5.3 \pm 0.8) \times 10^7$ | rt | Ad-33 | | Monr.79A05 |
| 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 | $K_d = 1.67 \times 10^{-3} \text{ [1.5]}.$ S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_d = 1.67 \times 10^4 \text{ s}^{-1}$ [1.5]. | Monr.79A05 |
| 10.68 | Ni(II) bis[$p-t$ - butylphenylsalicylate] | CCl ₄ /CHCl ₃ (9:1) v:v | 1.5×10^7 | rt | Ad-23 | $k_d = 1.67 \times 10^{-3} \text{ (1.5)}.$ S = A = Rub. Measured $k_Q/(k_A[A] + k_d) = 8.5 \times 10^3$ $dm^3 \text{ mol}^{-1} \text{ at } [A] = 5 \times 10^{-6}$ $mol \ dm^{-3}. \ k_Q \ derived \ using$ $k_A = 7 \times 10^7 \ dm^3 \ mol^{-1} \ s^{-1}$ and $k_d = 1.43 \times 10^3 \ s^{-1} \ [1.8].$ | Hrdl74F64 |
| | 0 | | LIGANDS 10.69 - | 10.70 : | | | |
| | | | 5 4 3 C(OH)=0 | = L | | | |
| 10.69 | Co(II) bis[3,5- diisopropyl- salicylate] $[R_3 = R_5 = -i-Pr]$ | C ₆ H ₅ CH ₃ | 3.0×10^7 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| 10.70 | $[R_3 - R_5 - i-Pr]$ Ni(II) bis[3,5-di- isopropylsalicylate] $[R_3 - R_5 - i-Pr]$ | C ₆ H ₅ CH ₃ | 5.0 × 10 ⁷ (est) LIGANDS 10.71 - | rt 10.75 : | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| | | | R' | = L | | | |
| 10.71 | Ni(II) bis(salycil- aldehyde oxime) | C ₆ H ₅ CH ₃ | 5.9×10^{9} (est) | rt | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| 10.72 | Ni(II) bis(2'- hydroxyaceto- phenone oxime) [R = ~Me] | C ₆ H ₅ CH ₃ | 5.2 × 10° (est) | rt | Ad-25 | $k_A = 1.7 \times 10^{4} \text{ In Initial S}$ $S = A = \text{Rub. } k \text{ estimated using } k_d = 1 \times 10^5 \text{ s}^{-1} \text{ (calc) and } k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}.$ | Zwei.75P063 |
| 10.73 | Ni(II) bis[2'- hydroxy-4'-methyl- acetophenone oxime] $\{R = R' = -Me\}$ | C ₆ H 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 | $\{K = K = -Me\}$ | C_6H_6 | $(3.1 \pm 0.3) \times 10^9$ | rt | Ad-8 | S = MB, $A = DPBF$, ruby laser | Wilk76F902 |
| 10.74 | Pd(II) bis [2'- hydroxy-4'-t-butyl- octadecanophenone oxime] | | $(6.0 \pm 0.5) \times 10^7$ | 25 | Ad-8 | (347 nm). S = An, A = DPBF, ruby laser (694 nm). | Farm.73F438 |
| 10.75 | [R = -heptadecyl, R' = -t-Ni(II) bis[2'-hydroxy-4'-methyl-dodecanophenone oxime] [R = -undecyl, R' = -Me] | C ₆ H 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 ₆ H 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 ₆ H ₅ CH ₃ | 5.7×10^9 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1} \text{ (calc)}$ and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| | | | LIGANDS 10.76 - | - 10.91 | | | |
| | | | R CH=NR | =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.79A0 |
| 10.77 | Ni(II) bis[$o-N$ -phenyl-aminoformimidoyl-phenol] [$R = -NHC_6H_5$] | C ₆ H ₅ CH ₃ | 7.5×10^9 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 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 $k_A = 5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [3.63.3]$ and $k_d = 1.67 \times 10^4 \text{ s}^{-1} [1.5]$. | Mon.79A05 |
| 10.78.1 | | C ₆ H ₅ CH ₃ | 5.9 × 10 ⁹ (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 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 | | Monr.79A0 |
| 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 | Monr.79A0: |
| 0.81 | 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 | [1.5]. S = A = Rub. k derived using $k_A = 5.3 \times 10^7$ $dm^3 mol^{-1} s^{-1} [3.63.3]$ and $k_d = 1.67 \times 10^4 s^{-1}$ | Monr.79A0 |
| 10.81.1 | | CH ₂ Cl ₂ | $ > 1.0 \times 10^9 $ (est) | 25 | Ad-23 | [1.5]. $S = A = Rub. k \text{ estimated using } k_A = 7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 7.3 \times 10^3 \text{ s}^{-1}$. | Carl72F31 |
| 10.81.2 | • | CH ₂ Cl ₂ | 2.0×10^9 (est) | 25 | Ad-23 | $S = A = Rub$. k estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and | Carl74F34 |
| 10.81.3 | 4 | i-octane | 2.6×10^9 (est) | 25 | Ad-23 | $k_{\rm d} = 8 \times 10^3 {\rm s}^{-1}$. $S = A = {\rm Rub.} \ k \ {\rm estimated \ using}$ $k_{\rm A} = 7.3 \times 10^7 {\rm dm}^3 {\rm mol}^{-1} {\rm s}^{-1}$ and $k_{\rm d} = 4.7 \times 10^4 {\rm s}^{-1} [1(a).6.1]$. | Carl74F34 |
| 10.81.4 | | i-octane | 2.4 × 10 ⁹ (est) | 25 | Ad-23 | | Carl.74F642 |
| 10.81.5 | | i-octane | 2.4×10^9 (est) | rt | Ad-23 | | Carl73P06 |
| 10.81.6 | | i-octane | 4.0×10^{9} (est) | 25 | Ad-23 | $k_d = 4.0 \times 10^{\circ} \text{ s} \ [1(a), 6].$ S = A = Rub. k estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ and}$ $k_d = 4.0 \times 10^4 \text{ s}^{-1} [1(a), 6].$ | Carl.74F642 |

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

| No. | Substrate (Q) | Solvent | $k_{\rm q}$ $'{ m dm}^3~{ m mol}^{-1}~{ m s}^{-1}$ | t /°C | Method | Comments | Ref. |
|---------|---|---|--|----------|--------|--|--------------|
| 10.81.7 | | hexadecane | 2.0 × 10 ⁸ (est) | 25 | Ad-33 | A = Rub. k estimated using k_A = $7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ | Carl72F31 |
| 10.81.8 | | hexadecane | 4.0×10^8 (est) | 25 | Ad-33 | and $k_d = 9.0 \times 10^4 \text{ s}^{-1}$ [I(a). 7]. ${}^{1}\text{O}_{2}^{*}$ from a microwave discharge, $A = \text{Rub. } k \text{ estimated using } k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ and } k_d = 9.0 \times 10^4 \text{ s}^{-1}$ [I(a). 7]. | Carl74F34 |
| 10.81.9 | | i-octane/ MeOH/ C ₅ H ₅ N (94:3:3) v:v:v | 3.5×10^9 (est) | 25 | Ad-32 | | Carl., 72F31 |
| 10.82 | Ni(II) bis[o-(N- sec-butylformimidoyl)- phenol] [R = -sec-Bu] | C ₆ H ₅ CH ₃ | 4.0×10^9 (est) | rt | Ad-25 | | Zwei.75P06. |
| 10.83 | Ni(II) bis[o -(N - t - butylformimidoyl)- phenol] [$R = -t$ -Bu] | C ₆ H 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] $[R = -cyclo-C_{e}H_{11}]$ | C ₆ H ₅ CH ₃ | 4.7×10^9 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{dm}^3 \text{mol}^{-1} \text{s}^{-1}$. | Zwei.75P06. |
| 10.85 | Co(II) bis[o-(N-phenylformimidoyl) phenol] [R = -Ph] | C ₆ H ₅ CH ₃ | 3.2×10^{9} (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.86 | Ni(II) bis[o-(N- phenylformimidoyl)- phenol] [R = -Ph] | C ₆ H ₅ CH ₃ | 7.8×10^9 (est) | rt | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.87 | Cu(II) bis[o-(N- phenylformimidoyl)- phenol] [R = -Ph] | C ₆ H ₅ CH ₃ | 4.0×10^{8} (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| 10.88 | Co(II) bis[o -(N - dodecylformimidoyl)- phenol] [$R = -n$ -dodecyl] | C ₆ H ₅ CH ₃ | 2.4×10^{9} (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| 10.89 | Ni(II) bis $\{o-(N-dodecylformimidoyl)-phenol\}$ $\{R = -n-dodecyl\}$ | C ₆ H ₅ CH ₃ | 7.0×10^9 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| 10.90 | Cu(II) bis[o-(N-dodecylformimidoyl)-phenol] | C ₆ H ₅ CH ₃ | 5.0×10^7 (est) | rt | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| 10.91 | [R = $-n$ -dodecyl] Ni(II)bis[o -(N -(p - anilinophenyl)- formimidoyl)phenol] [R = $-C_6H_4NHC_6H_5$] | C ₆ H ₅ CH ₃ | 1.7 × 10 ⁹ (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| | | | I IGANDS 10.02 - | 10.07. | | | |

LIGANDS 10.92 - 10.97:

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

| No. | Substrate (Q) | Solvent | $k_{\rm q}$ /dm ³ mol ⁻¹ s ⁻¹ | t /°C | Method | Comments | Ref. |
|--------|---|---|--|-------------------------|--------|---|-------------|
| 10.92 | Co(II) 2,2'-[ethyl- enebis(nitrilo- methylidyne)] diphenol | C ₆ H ₅ CH ₃ | 1.0×10^{10} (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06. |
| 10.93 | [R = -CH ₂ CH ₂ -, R" = -I Ni(II) 2,2'-[ethyl- enebis(nitrilo- methylidyne)] diphenol | C ₆ H ₅ CH ₃ | 5.3 × 10 ⁹ (est) | rt | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.94 | [R = -CH ₂ CH ₂ -, R" = -] Ni(II) 2,2'-[ethyl- enebis(nitrilo- ethylidyne)] diphenol | C ₆ H ₅ CH ₃ | 3.4×10^9 (est) | rt | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.95 | $[R = -CH_2CH_2-, R'' = -CN_1(II) 2,2'-[ethylene-bis(nitrilodecylidyne)]$ $di-p-cresol$ $[R = -CH_2CH_2-,$ $R'' = n-C_9H_{19}]$ | C ₆ H ₅ CH ₃ | 4.8 × 10 ⁹ (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06. |
| 10.96 | Ni(II) 2,2'-[o -phenylene- bis(nitrilomethyli- dyne)]diphenol [$R = -C_oH_4$ -, $R'' = -H$] | C ₆ H ₅ CH ₃ | 3.7×10^9 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_{\rm d} = 1 \times 10^5 {\rm s}^{-1}$ (calc) and $k_{\rm A} = 1.7 \times 10^8 {\rm dm}^3 {\rm mol}^{-1} {\rm s}^{-1}$. | Zwei.75P06. |
| 10.97 | Ni(II) 2,2'-[1,8- naphthylenebis- (nitrilomethyli- dyne)]diphenol $[R = -C_{10}H_6-, R'' = -H]$ | C ₆ H ₅ CH ₃ | 1.2×10^{10} (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| | $[K = -C_{10}\Pi_6^-, K = -\Pi]$ | | LIGANDS 10.98 | - 10.114 : | | | |
| | | | 5 6 | 0 ^Θ S ≡ L | | | |
| 10.98 | Ni(II) aquo[2,2'- thiobis(4- t - octyl)phenolate] [$R_4 = -t$ -octyl] | C ₆ H ₅ CH ₃ | 1.4×10^{8} (est) | rt | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.99 | Ni(II) aquo[2,2'- thiobis(3,4- dimethyl)phenolate] $[R_3 = R_4 = -Me]$ | C ₆ H ₅ CH ₃ | 1.2 × 10 ⁸ (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06. |
| 10.100 | Ni(II) ammine[2,2'- thiobis(4-t- octyl)phenolate] $[R_4 = -t$ -octyl] | C ₆ H ₅ CH ₃ | 4.8 × 10 ⁸ (est) | rt | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.101 | Ni(II) ethylamine [2,2'-thiobis(4- t -octyl)phenolate] [$\mathbf{R}_4 = -t$ -octyl] | C ₆ H ₅ CH ₃ | 3.1×10^{8} (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.102 | • • | C ₆ H ₅ CH ₃ | 4.1×10^8 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |

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

| No. | Substrate (Q) | Solvent | $k_{\rm q}$ /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 ₆ H ₅ CH ₃ | 3.0 × 10 ⁸ (est) | rt | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P063 |
| 10.104 | Co(II) n -butyl- amine[2,2'-thiobis- (4- t -octyl)phenolate] [$R_4 = -t$ -octyl] | C ₆ H ₅ CH ₃ | 3.7×10^8 (est) | rt | Ad-25 | S = A' = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1} \text{ (calc)}$ and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | 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.79A05 |
| 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 | | C₃H₃Br | 1.3 × 10 ⁸ | 0 | Ad-33 | $^{1}O_{2}$ * from microwave discharge, A = Rub. Measured $k_{Q}/[(k_{d}/[A]) + k_{A}] = 1.0$ 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]. Q exists as a tetramer in solution. | Guil.73F333 |
| 10.105.3 | | 2-butoxy- ethanol | 2.8×10^8 (est) | 0 | Ad-33 | $^{1}O_{2}^{*}$ from microwave discharge, A = Rub. k estimated using $k_{A} = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{d} = 3.8 \times 10^{5} \text{ s}^{-1} [I(a). 4].$ | Carl72F319 |
| 10.105.4 | | C ₆ H ₅ CH ₃ | 4.0×10^8 (est) | rt | Ad-25 | = | Zwei.75P063 |
| 10.105.5 | | i-octane | 1.8×10^8 (est) | 25 | Ad-23 | | Carl72F319 |
| 10.105.6 | | i-octane | 2.0×10^8 (est) | 25 | Ad-23 | S = A = Rub. k estimated using $k_A = 7.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 4.7 \times 10^4 \text{ s}^{-1} [1(a).6.1]$. | Carl74F341 |
| 10.105.7 | | i-octane | 1.4×10^8 (est) | 25 | Ad-23 | | Carl.74F642 |
| 10.105.8 | | hexadecane | 8.0×10^7 (est) | 25 | Ad-33 | 1 O ₂ * from microwave discharge, A = Rub. k estimated using $k_{A} = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{d} = 9.0 \times 10^{4} \text{ s}^{-1} [1(a).7]$. | Carl72F319 |
| 10.105.9 | | hexadecane | 1.0×10^{8} (est) | 25 | Ad-33 | $^{1}O_{2}^{*}$ from microwave discharge, A = Rub. k estimated using $k_{A} = 7.3 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1} \text{ and}$ $k_{d} = 9.0 \times 10^{4} \text{ s}^{-1} [I(a). 7].$ | Carl74F341 |
| 10.105.1 | | CCl ₄ /CHCl ₃ (9:1) v:v | 1.08×10^{8} | rt | Ad-23 | $k_{\rm d} = 1.03$ [110,17] $S = A = {\rm Rub. Measured}$ $k_{\rm Q}/(k_{\rm A}[{\rm A}] + k_{\rm d}) = 6.1 \times 10^4$ ${\rm dm^3 mol^{-1}}$ at $[{\rm A}] = 5 \times 10^{-6}$ ${\rm mol dm^{-3}}$. $k_{\rm Q}$ derived using $k_{\rm A} = 7 \times 10^7 {\rm dm^3 mol^{-1}} {\rm s^{-1}}$ and $k_{\rm d} = 1.43 \times 10^3 {\rm s^{-1}}$ [1.8]. | Hrdl74F64 |
| 10.105.1 | 1 | CS ₂ /MeOH (98:2) v:v | $(1.5 \pm 0.8) \times 10^8$ | rt | Ad-5 | S = MB, A = DPBF, flash photolysis. | Floo73F334 |
| 10.105.1 | 2 | <i>i</i> -octane/ MeOH/C₅H (94:3:3) v:v: | - | 25 | Ad-32 | $^{1}O_{2}^{*}$ from (PhO) ₃ PO ₃ decomp., A = Rub. k estimated using $k_{A} = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{d} = 5.0 \times 10^{4} \text{ s}^{-1}$. | Carl72F319 |

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

| No. | Substrate (Q) | Solvent / | $k_{\rm q}$ ${ m dm}^3~{ m mol}^{-1}~{ m s}^{-1}$ | t /°C | Method | Comments | Ref. |
|----------|--|---|---|----------|--------|--|------------|
| 10.106 | Ni(II) butyl- amine[2,2'-thiobis- (3,4-dimethyl)phenolate] [R ₃ = R ₄ = -Me] | C ₆ H ₅ CH ₃ | 2.5 × 10 ⁸ (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.107 | Ni(II) cyclohexyl- amine[2,2'-thiobis- (4-t-octyl)phenolate] $[R_4 = -t-\text{octyl}]$ | C ₆ H ₅ CH ₃ | 1.8 × 10 ⁸ (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1} \text{ (calc)}$ and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.108 | Ni(II) cyclo- hexylamine [2,2'-thiobis- (3,4-dimethyl)phenolate] $[R_3 = R_4 = -Me]$ | C ₆ H ₅ CH ₃ | 3.4×10^{8} (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1} \text{ (calc)}$ and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.109 | Ni(II) aniline[2,2'- thiobis(4- t -octyl)- phenolate] [$R_4 = -t$ -octyl] | C ₆ H ₅ CH ₃ | 1.9×10^8 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.110 | Ni(II) dodecyl- amine[2,2'-thiobis- (4-t-octyl)phenolate] $[R_4 = -t$ -octyl] | C ₆ H ₅ CH ₃ | 2.6×10^8 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{dm}^3 \text{mol}^{-1} \text{s}^{-1}$. | Zwei.75P06 |
| 10.111 | Ni(II) dodecylamine [2,2'-thiobis- (3,4-dimethyl)phenolate] $[R_3 = R_4 = -Me]$ | C ₆ H ₅ CH ₃ | 3.9×10^8 (est) | , rt | Ad-25 | $S = A = Rub. k$ estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 0.112 | Ni(II) didodecyl- amine[2,2'-thiobis- 3,4-dimethyl)phenolate] [R ₃ = R ₄ = -Me] | C ₆ H ₅ CH ₃ | 3.2×10^8 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.113 | Ni(II) triethanol- amine[2,2'-thiobis- (4-t-octyl)phenolate] $[R_4 = -t-\text{octyl}]$ | C ₆ H ₅ CH ₃ | 1.1×10^8 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 0.114 | 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 |
| 0.114. | 1 | C ₆ H ₅ Br | 3.9×10^7 | 0 | Ad-33 | $^{1}\text{O}_{2}$ * from microwave discharge, A = Rub. Measured $k_{\text{Q}}/[(k_{\text{d}}/[\text{A}]) + k_{\text{A}}] = 0.3 \text{ at } [\text{A}] = 1.5 \times 10^{-4} \text{ mol dm}^{-3}$. k_{Q} derived using $k_{\text{A}} = 4.0 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{\text{d}} = 1.3 \times 10^{4} \text{ s}^{-1} [1.34]$. | Guil.73F33 |
| 10.114.: | 2 | C ₆ H ₅ CH ₃ | 2.7×10^8 (est) | rt | Ad-25 | S = A = Rub. k estimated using $k_d = 1 \times 10^5 \text{ s}^{-1}$ (calc) and $k_A = 1.7 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Zwei.75P06 |
| 10.114. | | i-octane | 1.3×10^8 (est) | 25 | Ad-23 | S = A = Rub. k estimated using $k_A = 7 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 4.0 \times 10^4 \text{ s}^{-1} [I(a).6]$. | Carl72F3 |
| 10.114. | 4 | i-octane | 9.6×10^7 (est) | 25 | Ad-23 | | Carl74F34 |
| 0.114. | 5 | hexadecane | 1.3×10^{8} (est) | 25 | Ad-33 | $^{1}\text{O}_{2}$ * from microwave discharge, A = Rub. k estimated using $k_{A} = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{d} = 9.0 \times 10^{4} \text{ s}^{-1} [1(a).7]$. | Carl72F3 |
| 0.114. | 6 | CCl ₄ /CHCl ₂ (9:1) v:v | $_{3}$ 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 $[A] = 5 \times 10^{-6}$ mol dm^{-3} . k_Q derived using $k_A = 7 \times 10^7 dm^3 mol^{-1}$ s ⁻¹ and $k_d = 1.43 \times 10^3 s^{-1} \{1.8\}$. | Hrdl74F€ |

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

| No. | Substrate (Q) | Solvent | $k_{\rm q}$ $/{\rm dm}^3 \ {\rm mol}^{-1} \ {\rm s}^{-1}$ | /°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. | Floo73F334 |
| 10.114.8 | 3 | <i>i</i> -octane/ MeOH/ C ₅ H ₅ N (94:3:3) v:v: | 2.0×10^{8} (est) | 25 | Ad-32 | $^{1}O_{2}^{*}$ from (PhO) ₃ PO ₃ decomp., A = Rub. k estimated using $k_{A} = 7 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{d} = 5.0 \times 10^{4} \text{ s}^{-1}$. | Carl72F319 |
| 10.115 | Ni(II) bis[1,3-bis (2-pyridylimino) isoindoline] | CHCl ₃ | $(1.6 \pm 0.3) \times 10^8$ | rt | Ad-33 | | Monr.79A050 |
| | N N N N N N N N N N N N N N N N N N N | | | | | | |
| 10.116 | (3,11-bisacetyl-4,10-dimethyl-1,5,9,13-tetraazacyclo-pentadeca-1,3,9,11-tetraene- <i>N</i> , <i>N</i> ', <i>N</i> '', <i>N</i> ''') Ni(II) | снсі, | $(1.6 \pm 0.3) \times 10^9$ | 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 |
| | H ² C CH ² N N CH ² CH ³ CH | •L | | | | | |

LIGANDS 10.117 -10.121:

10.118

10.119

10.119.1

10.121

tetraphenylporphine

10.117 Ni(II) tetraphenyl-
$$CCl_4$$
 (2.0 ± 0.6) × 10⁹ rt Ld-13 S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1} [1.8.3]$.

10.118 Cu(II) tetraphenyl- CCl_4 (5.0 ± 1.5) × 10⁶ rt Ld-13 S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1} [1.8.3]$.

10.119 Zn(II) tetraphenyl- CCl_4 (4.0 ± 1.2) × 10⁷ rt Ld-13 S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1} [1.8.3]$.

10.119.1 CCl_4 (4.0 ± 1.2) × 10⁷ rt Ld-13 S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1} [1.8.3]$.

10.119.1 CCl_4 $k_r = 1$ rt Ad-27 S = ? k_r derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1} [1.8.3]$.

10.120 $Co(III)$ tetraphenyl- CCl_4 (2.0 ± 0.6) × 10⁹ rt Ld-13 S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1} [1.8.3]$.

10.121 acetate-Fe(III)- CCl_4 (1.5 ± 0.5) × 10⁹ rt Ld-13 S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1} [1.8.3]$.

 $k_{\rm d} = 3.6 \times 10^1 \, {\rm s}^{-1} [1.8.3].$

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

| No. | Substrate (Q) | Solvent / | $k_{\rm q}$ ${\rm dm}^3~{\rm mol}^{-1}~{\rm s}^{-1}$ | t ∕°C | Method | Comments | Ref. |
|---------|-----------------------------------|-------------------------|--|----------|--------|--|-------------|
| 10.122 | Zn(II) tetraphenyl- chlorin | CCl₄ | $(4.0 \pm 1.2) \times 10^9$ | rt | Ld-13 | $S = ? k$ derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1} \{1.8.3\}.$ | Kras79A010 |
| 10.122. | 1 | CCl₄ | $k_{\rm r} = (2.0 \pm 1.4) \times 10^8$ | rt | Ad-27 | S = ? k derived using $k_A = 4.0 \times 10^9 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [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 |
| | Θ ■L | | | | | | |
| 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 | CCl₄/CHCl₃ (9:1) v:v | 3.0×10^6 | rt | Ad-23 | • , | Hrdl74F64: |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------------|---|-------------------|--|---------------------------------------|-----------|--------|--|-------------|
| , | | | | ill rate constant unless | | | | |
| 11.1 | 1-butanthiol CH ₃ (CH ₂) ₂ CH ₂ SH | MeOH | thing rate constant) is 5.9×10^4 | specified; k_d is the rate 1.7 | rt | | S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ | Mart72F519 |
| 11.2 | benzylmercaptan C ₆ H ₅ CH ₂ SH | МеОН | 1.4 × 10 ⁵ | 7.3×10^{-1} | rt | A'd-16 | [1.3.6]. S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. | Mart72F519 |
| 11.3 | butylmethyl sulfide CH ₃ (CH ₂) ₂ CH ₂ SCH | CHCl ₃ | $(2.9 \pm 0.3) \times 10^7$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ 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 ₆ H ₅ SCH ₃ | МеОН | $(2.0 \pm 0.1) \times 10^6$ | | 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 |
| 11.4.1 | | 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 ₆ H ₅ CH ₂ SCH ₃ | CHCl ₃ | $(1.2 \pm 0.2) \times 10^7$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_d = 1.7 \times 10^4$ s ⁻¹ [1.5]. | Monr79A085 |
| | | | | COMPOUNDS 11.6 | 5 - 11.13 | : | | |
| | | | | CH ₃ S - 2 3 | • | | | |
| 11.6 | methyl-4-fluoro- phenyl sulfide $[\mathbf{R}_4 = -\mathbf{F}]$ | CHCl ₃ | $(1.9 \pm 0.2) \times 10^6$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ 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 $k_{A'} = 5.3 \times 10^7$ dm³ 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 $[R_4 = -Cl]$ | МеОН | $(8.25 \pm 0.5) \times 10^5$ | | rt | A'd-16 | S = RB, A' = DPF. k derived using k_d = $1.1 \times 10^5 \text{ s}^{-1}$ [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 | • • | Monr79A085 |

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

| No. S | Substrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|--|-------------------------------|--|---------------------------------------|----------|--------|---|---------------|
| 11.10 | methyl-3-methyl- phenyl sulfide [R ₃ = -CH ₃] | CHCl ₃ | $(3.1 \pm 0.4) \times 10^6$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_d = 1.7 \times 10^4$ s ⁻¹ [1.5]. | Monr79A085 |
| 11.11 | methyl-4-methyl- phenyl sulfide $[R_4 = -CH_3]$ | MeOH | $(3.1 \pm 0.2) \times 10^6$ | | 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 |
| 11.11.1 | | CHCl ₃ | $(4.6 \pm 0.5) \times 10^6$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_d = 1.7 \times 10^4$ s ⁻¹ [1.5]. | Monr79A085 |
| 11.12 | methyl-4-methoxy- phenyl sulfide [R ₄ = -OCH ₃] | - МеОН | $(5.3 \pm 0.2) \times 10^6$ | | 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 |
| 11.12.1 | I | CHCl ₃ | $(7.6 \pm 0.8) \times 10^6$ | | 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 |
| 11.13 | methyl-4- t -butyl phenyl sulfide $[R_4 = -C(CH_3)_3]$ | CHCl ₃ | $(4.7 \pm 0.5) \times 10^6$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_d = 1.7 \times 10^4$ s ⁻¹ [1.5]. | Monr79A085 |
| 11.14 | diethyl sulfide (C ₂ H ₅) ₂ S | МеОН | 4.8 × 10 ⁶ | $(2.1 \pm 0.6) \times 10^{-2}$ | rt | Pa-15 | S = ZnTPP. k derived using $k_d = *1.0 \times 10^5$ s^{-1} [1.3.6]. | Foot.71F580 |
| 11.14.1 | | МеОН | $(1.71 \pm 0.06) \times 10^7$ | | 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 |
| 11.14.2 | | C ₆ H ₆ | 1.3×10^{6} | $(3.2 \pm 0.5) \times 10^{-2}$ | rt | Pa-15 | S = ZnTPP. k derived using $k_d = *4.0 \times 10^4$ s ⁻¹ [1.32.9]. | Foot.71F580 |
| 11.14.3 | 3 | C ₆ H 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 | 4 | C ₆ H ₆ | 7.6×10^6 | | rt | Pa-20 | S = ZnTPP, A' = Car. Measured $k_A/(k_d + k[A])$ $(1.74 \pm 0.05) \times 10^4 \text{ dm}^3$ mol ⁻¹ at [A] = 0.1 mol dm k derived using $k_{A'}$ = *1.3 × 10 ¹⁰ dm ³ mol ⁻¹ s ⁻¹ [2.130.12] and k_d = | |
| 11.14. | 5 | C₀H₀ | $(2.0 \pm 0.2) \times 10^7$ | | rt | A'd-16 | *4.0 × 10 ⁴ s ⁻¹ [1.32.9]. S = ZnTPP, A' = DPF. Iderived using k_d = *4.0 × 10 ⁴ s ⁻¹ [1.32.9]. Error is a 95% confidence limit. | k Kach.79A086 |

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

| No. S | Substrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|--|---|--|---------------------------------------|----------|--------|--|-------------|
| 11.14.6 | j | C ₆ H ₆ /MeOH (4:1)v:v | 6.0×10^{6} *2.3 × 10 ⁶ $k_{\rm r} = 3 \times 10^{5}$ | 1 | 25 | P'a-20 | S = MB, A' = 2M2P, P = diethylsulfoxide. k derived using $\beta_{A'} = 4.0 \times 10^{-2}$ | Foot70F734 |
| | | | | | | | mol dm ⁻³ and $k_d = 1.0 \times 10^5$ (*3.8 × 10 ⁴) s ⁻¹ (calc). | |
| 11.15 | t-butylethyl sulfide CH ₃ CH ₂ SC(CH ₃) ₃ | CHCl ₃ | $(6.4 \pm 0.7) \times 10^6$ | | rt | A'd-33 | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ 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] ₂ S | МеОН | 4.0 × 10 ⁶ | 2.5×10^{-2} | 20 | Od-15 | S = RB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a =$ 5.4 kJ mol ⁻¹ . | Koch68F288 |
| 11.16.1 | , | МеОН | 7.7×10^{6} | 1.3×10^{-2} | 20 | Od-15 | | Koch68F288 |
| 11,16.2 | | МеОН | 6.3 × 10 ⁶ | 1.6×10^{-2} | 20 | Od-15 | | Koch68F288 |
| 11.16.3 | | MeOH | 4.5×10^6 | 2.2×10^{-2} | 20 | Od-15 | - | Koch68F288 |
| 11.16.4 | | МеОН | 1.0×10^7 | 1.0×10^{-2} | 20 | Od-15 | | Koch68F288 |
| 11.17 | diisopropyl sulfide [(CH ₃) ₂ CH] ₂ S | МеОН | $(2.51 \pm 0.03) \times 10^6$ | | rt | A'd-16 | $S = RB$, $A' = DPF$. k derived using $k_d = 1.1 \times 10^5 \text{ s}^{-1}$ [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 | | S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ 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 ₃ CH ₂ CH(CH ₃)Se | CHCl ₃ CH ₂ CH ₂ CH | $(1.1 \pm 0.2) \times 10^7$ \mathbf{f}_3 | | 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 $k_d = 1.7 \times 10^4$ | Monr79A085 |
| 11.19 | t-butylpropyl sulfide (CH ₃) ₃ CSCH ₂ CH ₂ C | CHCl ₃ | $(7.2 \pm 0.8) \times 10^6$ | | rt | A'd-33 | s^{-1} [1.5]. S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ $dm^3 mol^{-1} s^{-1}$ [3.63.3] and $k_d = 1.7 \times 10^4$ | Monr79A085 |
| 11.20 | dibutyl sulfide [CH ₃ (CH ₂) ₂ CH ₂] ₂ S | МеОН | 9.1×10^6 | 1.1×10^{-2} | rt | A'd-16 | s^{-1} [1.5]. S = MB, $A' = DPBF$. k derived using $k_d = *1.0 \times 10^5 s^{-1}$ [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 | $\beta (k_d/k)$ /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 $k_{A'} = 5.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_d = 1.7 \times 10^4$ s ⁻¹ [1.5]. | Monr79A085 |
| 11.20.2 | EtOH | $k_{\rm r}=5.4\times10^6$ | | 25 | ? | S = chrysene, 2-bromo- chrysene, MB. Measured $(k_q/k_r) \approx 0.7$. k_r derived using $k_A(\text{MeOH}) = 9.1 \times$ | Casa74F648 |
| 11.21 di-2-butyl sulfide [CH ₃ CH ₂ C(CH ₃)] ₂ S | CHCl ₃ | $(1.8 \pm 0.2) \times 10^6$ | | rt | A'd-33 | dm³ mol ⁻¹ s ⁻¹ [11.20]. S = A' = Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_d = 1.7 \times 10^4$ s ⁻¹ [1.5]. | Monr79A085 |
| di-t-butyl sulfide [(CH ₃) ₃ C] ₂ S | МеОН | ~1.5 × 10 ⁵ | | rt | A'd-16 | S = RB, A' = DPF. k derived using k_d = 1.1×10^5 s ⁻¹ [1.3.4]. Theoretical intercept of | Kach.79A086 |
| 11.22.1 | CHCl ₃ | $(1.3 \pm 0.3) \times 10^5$ | | rt | A'd-33 | 1.0 used in calculation. $S = A' = Rub. k$ 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 $(C_6H_5)_2S$ | МеОН | ~1.0 × 10 ⁵ | | rt | A'd-16 | S = RB, A' = DPF. k derived using k_d = 1.1 × 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 ₆ H ₅ CH ₂) ₂ S | МеОН | 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]. $E_a = 3.8 \text{ kJ mol}^{-1}$. | Koch68F288 |
| 11.24.1 | МеОН | 1.5×10^7 | 6.7×10^{-3} | 20 | Od-15 | S = tetrachloroeosin. $k \text{ derived using } k_d = $ *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. $E_a = 5.4 \text{ kJ mol}^{-1}$. | Koch68F288 |
| 11.24.2 | МеОН | 1.8×10^7 | 5.5×10^{-3} | 20 | Od-15 | $E_a = 5.4 \text{ kJ mol}^{-1}$. S = tetrachloro- fluorescein. k derived using $k_d =$ *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. $E_a = 1.7 \text{ kJ mol}^{-1}$. | Koch68F288 |
| 11.24.3 | МеОН | 1.1×10^7 | 9.0×10^{-3} | 20 | Od-15 | | 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. S | Substrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_{d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|--|------------------------------|--|---|----------|--------|---|-------------|
| 11.25 | tetrahydro- thiophene | МеОН | 3.1 × 10 ⁶ | 3.2 × 10 ⁻² | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [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 $k_{A'} = 5.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_d = 1.7 \times 10^4$ 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 $k_{A'} = 5.3 \times 10^7$ dm ³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_d = 1.7 \times 10^4$ s ⁻¹ [1.5]. | Monr79A085 |
| 11.27 | 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 $k_{A'} = 5.3 \times 10^7$ dm ³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_{d} = 1.7 \times 10^4$ s ⁻¹ [1.5]. | Monr79A085 |
| 11.28 | 1-thiacyclo- heptane | CHCl ₃ | $(1.3 \pm 0.2) \times 10^7$ | | rt | A'd-33 | S = A' Rub. k derived using $k_{A'} = 5.3 \times 10^7$ dm³ mol ⁻¹ s ⁻¹ [3.63.3] and $k_{d} = 1.7 \times 10^4$ s ⁻¹ [1.5]. | Monr79A085 |
| 11.29 | thiourea (NH ₂) ₂ CS | H ₂ O (pH 7.1) | 4.4 × 10 ⁶ | | 25 | Od-19 | | Kral.78A360 |
| 11.29.1 | | МеОН | $2.5 	imes 10^6$ | 4.0×10^{-2} | 20 | Od-15 | S = MB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a =$ 6.3 kJ mol ⁻¹ . | Koch68F288 |
| 11.30 | N-methylthiourea CH ₃ NH(NH ₂)CS | H ₂ O (pH 7.1) | 2.0×10^6 | | 25 | Od-19 | S = phenosafranine, $Q = \text{NaN}_3$. k derived using $k_Q = 2.0 \times 10^8$ dm³ mol ⁻¹ s ⁻¹ [12.9.6]. | Kral.78A360 |
| 11.31 | N-allylthiourea CH ₂ =CHCH ₂ NH(| | 4.4 × 10 ⁸ | 9.9 × 10 ⁻⁴ | rt | Od-14 | | Sluy61F008 |
| 11.31.1 | | H ₂ O (pH 7.1) | 4.0 × 10 ⁶ | | 25 | Od-19 | • • | Kral.78F020 |
| 11.31.2 | | H ₂ O (pH 7.0) | 4.5×10^6 | | 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 (1.0 % by volume). | Barb.78A278 |
| 11.31.3 | | МеОН | 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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|---|--|--|----------|-----------------------|--|---------------|
| 11.31. | 4 | C ₅ H ₅ N | $\approx 2.7 \times 10^7$ | | 12 | P'a-20 | $S = A' = DMA$. Measured $(k/k_A) = 0.7$. k derived using $(k(TME)/k_A) = 1.1$ and $k(TME) = 4.0 \times 10^7$ | i Kram.73F202 |
| | | | | COMPOUNDS 11.3 | 2 – 11.3 | 4 : | $dm^3 mol^{-1} s^{-1} [2.35.3].$ | |
| | | | | 5 0 2 5 0 3 | | , | | |
| 11.32 | 4H-pyran-4- thione | CH ₂ Cl ₂ | 7.5×10^6 | $(1.6 \pm 0.5) \times 10^{-3}$ | 25 | Pa-15 | S = MB, $P = 4H$ -pyran- 4-ketone. k derived using $k_d =$ | Ishi71F403 |
| 11.33 | 2,6-dimethyl- 4H-pyran-4-thione $[R_2 = R_6 = -Me]$ | CH ₂ Cl ₂ | 4.0 × 10 ⁷ | $(3.0 \pm 0.9) \times 10^{-4}$ | 25 | Pa-15 | *1.2 \times 10 ⁴ s ⁻¹ [\bar{I} .4.2], S = MB, P = 2,6- dimethyl-4 <i>H</i> -pyran- 4-ketone. k derived using k_d = | Ishi71F403 |
| 11.34 | 2,6-diphenyl-4 H - pyran-4-thione [$R_2 = R_6 = -Ph$] | CH ₂ Cl ₂ | 8.6×10^6 | $(1.4 \pm 0.2) \times 10^{-3}$ | 25 | Ad-15 | *1.2 × 10 ⁴ s ⁻¹ [1.4.2]. S = MB, k derived using k_d = | Ishi71F403 |
| 11.35 | | МеОН | $\leq 1.7 \times 10^2$ | $\geqslant 6.0 \times 10^2$ | 20 | Od-15 | using $k_d = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6].$ | Koch68F288 |
| | (s) | | | • | | | $E_{\rm a}=25~{\rm kJ~mol^{-1}}.$ | |
| 11.35. | 1 | МеОН | 2.2×10^{5} | 4.5×10^{-1} | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ | Mart72F519 |
| | | | | COMPOUNDS 11.3 | 6 – 11.3 | 8: | [1.3.6]. | |
| | | | | 8 N N N N N N N N N N N N N N N N N N N | 2 3 | | | |
| 11.36 | phenothiazine $[R_{10} = -H]$ | MeOH /C ₆ H ₆ (9:1) v:v | 4.5 × 10 ⁷ | $\beta_{\tau} = 2.2 \times 10^{-3}$ (est) | 15 | Pa-17 P'a (sep) | S = MB, Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.94$. β_r estimated using $k_r = 4.2 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [11.36.5] and $k_d(\text{MeOH}) =$ | Ram75F623 |
| 11.36. | 1 | MeOH /C ₆ H ₆ (4:1) v:v | 2.6×10^{7} (est) | $ \beta_{\rm r} = 2.4 \times 10^{-3} $ (est) | 15 | Pa-17 P'a (sep) | *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. k_r derived using k_d = *1.0 × 10 ⁵ s ⁻¹ [1.3.6]. 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 = | Ram75F623 |

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

| No. Substrate (A) | Solvent | /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--|--|--|--|----------|-----------------------|---|-------------|
| 11.36.2 | MeOH /C ₆ H 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 $(\beta_r/\beta_r(\text{MeOH})) = 1.5$. β_r estimated using $k_r = 4.2 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ $[11.36.5] \text{ and } k_d(\text{MeOH}) = *1.0 \times 10^5 \text{ s}^{-1} [1.3.6]$. k_r estimated using $k_d = 6.12 \times 10^4 \text{ s}^{-1} (\text{col}_2)$ | Ram75F623 |
| 11.36.3 | MeOH /glycol (3:1) v:v | 9.2×10^{7} (est) | $\beta_{\rm r} = 1.2 \times 10^{-3}$ | 15 | Pa-17 P'a (sep) | 6.13 × 10 ⁴ s ⁻¹ (calc). S = MB. Measured (β_r/β_r (MeOH)) = 0.51. 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 = 1.1 × 10 ⁵ s ⁻¹ (calc). | Ram75F623 |
| 11.36.4 | MeOH /glycol (1:3) v:v | 1.8 × 10 ⁸ (est) | $\beta_{\rm r} = 8.0 \times 10^{-4}$ | 15 | Pa-17 P'a (sep) | S = MB. Measured $(\beta_r/\beta_r(\text{MeOH})) = 0.34$. β_r estimated using $k_r = 4.2 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [11.36.5] and $k_d(\text{MeOH}) = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6]. k_r estimated using $k_d = 1.4 \times 10^5 \text{ s}^{-1}$ (calc). | Ram75F623 |
| 11.36.5 | C ₆ H ₅ Br /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 | Rose77F240 |
| 11.37 10-methylpheno- thiazine $[R_{10} = -Me]$ | C ₆ H ₅ Br /MeOH (2:1) v:v | < 1.2 × 10 ⁶ (est) | | rt | A'd-23 | $k_d = 4.89 \times 10^4 \text{ s}^{-1} \text{ (calc)}.$ S = A' = Rub. k estimated using $k_{A'} = 4 \times 10^7$ $\text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1} \text{ and}$ $k_d = 4.89 \times 10^4 \text{ s}^{-1} \text{ (calc)}.$ | Rose77F240 |
| 11.38 chloropromazine $[R_3 = -Cl, R_{10} = -(CH_2)_3N(CH_3)_2]$ | C ₆ H ₅ Br /MeOH (2:1) v:v | 3.5×10^7 (est) | | rt | A'd-23 | S = A' = Rub. k estimated using $k_{A'}$ = $4 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = 4.89 \times 10^4 \text{ s}^{-1}$ (calc). | Rose77F240 |
| 11.39 diethyl disulfide C ₂ H ₅ SSC ₂ H ₅ | MeOH | 1.8×10^7 | 5.5 × 10 ⁻³ | rt | A'd-16 | S = MB, A' = DPBF. k derived using $k_d = *1.0 \times 10^5$ | Mart72F519 |
| 11.40 1,4-dithiane | CH₃CN | 5.1×10^5 | ~5.0 × 10 ⁻² | rt | Pa-15 | s ⁻¹ [1.3.6]. S = RB. k derived using $k_d = *2.55 \times 10^4$ s ⁻¹ [1.17]. Slope estimated as tangent to curve. | Foot.71F580 |
| 11.40.1 | CH ₃ CN | $2.6 	imes 10^6$ | $(9.8 \pm 0.7) \times 10^{-3}$ | rt | Pa-15 | S = RB. k derived using $k_d = *2.55 \times 10^4$ s ⁻¹ [1.17.2]. Solvent contained 0.05% H ₂ O by | Foot.71F580 |
| 11.40.2 | CH ₃ CN | 1.5×10^6 | $(1.7 \pm 0.2) \times 10^{-2}$ | rt | Pa-15 | molarity. S = RB. k derived using $k_d = *2.55 \times 10^4$ s^{-1} [1.17.2]. Solvent contained 0.52% H ₂ O by molarity. | Foot.71F580 |

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

| No. | Substrate (A) | Solvent | $\frac{k}{\text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------------------|---|---|---|---------------------------------------|----------|--------|--|--------------|
| 11.40.3 11.40.4 | | CH ₃ CN/H (95:5) Mole % | $_{2}O 6.3 \times 10^{6}$ (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 |
| | | CH ₃ CN/H (61:39) Mole % | $_{2}O 1.1 \times 10^{7}$ (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 | dimethyldithio- carbamate ion (CH ₃) ₂ NCSS ⁻ | H ₂ O (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 | hexamethylene- dithiocarbamate | EtOH | 1.5×10^8 | | rt | Od-23 | S = RB, A' = Car. Measured $k_{\rm A}/(k_{\rm d} + k_{\rm A})$ [A]) = 7 × 10 ⁴ dm ³ mol ⁻¹ at [A] = 3.35 × 10 ⁻⁴ mol dm ⁻³ . k derived using $k_{\rm A'} = 5.0 \times 10^9$ dm ³ mol ⁻¹ s ⁻¹ and $k_{\rm d} = 1.0 \times 10^4$ s ⁻¹ . | Yama.,72F116 |
| 11.43 | 4 <i>H</i> -thiopyran- 4-thione | CH ₂ Cl ₂ | > 1.2 × 10 ⁸ | < 1.0 × 10 ⁻⁴ | 25 | Pa-15 | S = MB, P = 4H- thiopyran-4-ketone. k derived using $k_d = *1.2 \times 10^4 \text{ s}^{-1}$ [1.4.2]. | Ishi71F403 |
| 11.44 | 2,6-diphenyl- 4 <i>H</i> -thiopyran- 4-thione | CH ₂ Cl 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]. | Ishi71F403 |
| | C _G H _S S C _G H _S | | | | | | | |
| 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 $k_d = 4.2 \times 10^4 \text{ s}^{-1}$ [1.32]. | Stev74F641 |
| | | | | For more relative rate | 25 500 | 3.63.2 | 0 | |
| 11.46 | 4,5-diphenyl 1,3-dithiole-2- thione | C ₆ H ₆ /MeOH (5:1) v:v | 3.6×10^7 (est) | 1.4×10^{-3} | 20 | | S = MB, k estimated using $k_d = 5.0 \times 10^4$ s ⁻¹ (calc). | Fang.77F794 |
| | C ₆ H ₅ | | | | | | | |
| 11.47 | 9-benzene- sulfonyl- 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 $k_d = 3.0 \times 10^4 \text{ s}^{-1}$ [1.25]. | Bete.70F250 |
| | SO ₂ C _e H ₅ | | | , | | | | |
| 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 $k_d = 3.0 \times 10^4 \text{ s}^{-1}$ [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 | $\beta (k_d/k)$ /mol dm ⁻³ | /°C | Method | Comments | Ref. |
|--------|---|---|--|---|-----|--------|---|-------------|
| | | | | ant unless k_r (chemical is the rate constant for | | | | |
| 12.1 | chloride ion [CH ₃ (CH ₂) ₂ CH ₂] ₄ NO | C ₆ H ₅ Br | ≤ 10 ⁶ | | rt | _ | S = A' = Rub. No measurable effect. ^a | Rose.76F126 |
| 12.1. | 1 | C ₆ H ₅ Br /MeO: (2:1) v:v | ≤ 10 ⁶ H | | rt | A'd-23 | S = A' = Rub. No measurable effect. ^a | Rose.76F126 |
| 12.2 | bromide ion LiBr | C_6H_5Br $/Me_2C$ $(2:1)$ v:v | ≤ 10 ⁶ CO | | rt | A'd-23 | S = A' = Rub. No measurable effect. ^a | Rose.76F126 |
| 12.2. | 1 | C_6H_5Br /MeOl (2:1) v:v | < 10 ⁶ H | | rt | A'd-23 | S = A' = Rub. No measurable effect. ^a | Rose.76F126 |
| 12.3 | bromide ion [CH ₃ (CH ₂) ₂ CH ₂] ₄ NE | C ₆ H ₅ Br Br /Me ₂ C | < 10 ⁶ | | rt | A'd-23 | S = A' = Rub. No measurable effect. ^a | Rose.76F126 |
| 12.3. | 1 | (2:1) v:v C ₆ H ₅ Br /MeOl (2:1) v:v | ≤ 10 ⁶ H | | rt | A'd-23 | S = A' = Rub. No measurable effect. ^a | Rose.76F126 |
| 12.4 | bromide ion (dicyclohexano-18- crown-6-poly- ether potassium bromide) | C ₆ H ₅ Br | $\approx 1.2 \times 10^6$ CO (est) | | rt | A'd-23 | S = A' = Rub. k estimated using $k_d = 3.24 \times 10^4 \text{ s}^{-1}$ (calc) and $k_{A'} = 4 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Rose.76F126 |
| 12.5 | iodide ion LiI | C ₆ H ₅ Br /Me ₂ C (2:1) v:v | $(8.1 \pm 0.1) \times 10^{-10}$ (est) | D ⁷ | rt | A'd-23 | S = A' = Rub. k estimated using $k_d = 3.24 \times 10^4 \text{ s}^{-1}$ (calc) and $k_{A'} = 4 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Rose.76F126 |
| 12.5. | 1 | C ₆ H ₅ Br /MeOI (2:1) v:v | ≼ 10 ⁶ H | | rt | A'd-23 | S = A' = Rub. No measurable effect. ^a | Rose.76F126 |
| 12.6 | iodide ion KI | H ₂ O | 7.2×10^6 | | 28 | Pa-23 | S = 1-anthracene- sulfonate ion, Q = NaN ₃ , P = I ₃ ⁻ . k derived using k_d = $5.0 \times 10^5 \text{ s}^{-1} [I.I]$ and k_Q = $2.2 \times 10^8 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [12.9.6]. | Roha.77F074 |
| 12.6. | I [*] | H ₂ O | 6.4×10^6 | | 28 | Pa-23 | S = 2-anthracene- sulfonate ion, Q = NaN ₃ , P = I ₃ . k derived using k_d = $5.0 \times 10^5 \text{ s}^{-1} [I.I]$ and k_Q = $2.2 \times 10^8 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [12.9.6]. | Roha.77F074 |
| 12.6.2 | 2 | H ₂ O | 7.2 × 10 ⁶ | | 28 | Pa-23 | find s [12.9.6]. S = 1,5-anthracene-disulfonate ion, Q = NaN ₃ , P = I ₃ ⁻ . k derived using k_d = $5.0 \times 10^5 \text{ s}^{-1} [1.1]$ and k_Q = $2.2 \times 10^8 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [12.9.6]. | Roha.77F074 |
| 12.6. | 3 | H ₂ O | 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 = $5.0 \times 10^5 \text{ s}^{-1}$ [1.1]. | Gupt.78F183 |

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

| No. Substrate (A) | Solvent | $/dm^3 \text{ mol}^{-1} \text{ s}^{-1}$ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--|--|---|---------------------------------------|----------|--------|--|-------------|
| 12.6.4 | H ₂ O/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 $k_d = 4.0 \times 10^5 \text{ s}^{-1}$ | Gupt.78F183 |
| 12.6.5 | H ₂ O/MeOH (3:2) v:v | 2.98×10 ⁶ (est) | 1.1 × 10 ⁻¹ | rt | Pa-23 | (calc). S = A' = 1-anthracene sulfonate, $Q = N_3$, $P = I_3$. k estimated using $k_d = 3.2 \times 10^5 \text{ s}^{-1}$ | Gupt.78F183 |
| 12.6.6 | H ₂ O/MeOH (2:3) v:v | (est) | 1.6×10^{-1} | rt | Pa-23 | (calc). S = A' = 1-anthracene sulfonate, $Q = N_3^-$, $P = I_3^-$. k estimated using $k_d = 2.5 \times 10^5 \text{ s}^{-1}$ (calc). | Gupt.78F183 |
| 12.6.7 | H ₂ O/MeOH (1:4) v:v | 3.4×10 ⁵ (est) | 5.6 × 10 ⁻¹ | rt | Pa-23 | (calc). S = A' = 1-anthracene sulfonate, $Q = N_3^-$, $P = I_3^-$. k estimated using $k_d = 1.9 \times 10^5 \text{ s}^{-1}$ (calc). | Gupt.78F183 |
| 12.6.8 | C ₆ H₅Br ∕MeOF (2:1) v:v | < 10 ⁶ I | | rt | A'd-23 | S = A' = Rub. No measurable effect. ^a | Rose.76F126 |
| 12.7 iodide ion [CH ₃ (CH ₂) ₂ (| C ₆ H ₅ Br | $(9.1 \pm 0.1) \times 10^7$ O (est) | | rt | A'd-23 | S = A' = Rub. k estimated using $k_d = 3.24 \times 10^4 \text{ s}^{-1}$ (calc) and $k_{A'} = 4 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Rose.76F126 |
| 12.7.1 | C ₆ H ₅ Br /MeOF (2:1) v:v | ≤ 10 ⁶ | | rt | A'd-23 | S = A' = Rub. No measurable effect. ^a | Rose.76F126 |
| 12.8 iodide ion (dicyclohex- crown-6-pc potassium io | C_6H_5Br ano-18- $/Me_2C_6$ olyether (2:1) v:v | $(2.8 \pm 0.1) \times 10^8$ O (est) | | rt | A'd-23 | S = A' = Rub. k estimated using $k_d = 3.24 \times 10^4 \text{ s}^{-1}$ (calc) and $k_{A'} = 4 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. | Rose.76F126 |
| 12.9 azide ion NaN ₃ | H ₂ O | 7.9×10^8 | | `40 | A'd-23 | S = Py, $A' = DPBF$. k derived using $k_d = 5.0 \times 10^5 \text{ s}^{-1} [I.I]$. A' and S solubilized in SDS micelles. | Miyo.78A174 |
| 12.9.1 | H ₂ O | 1.8 × 10° | | 40 | A'd-23 | $S = Py, A' = DPBF.$ $k \text{ derived using } k_d = 5.0 \times 10^5 \text{ s}^{-1} [I.I].$ A' and S solubilized in SDS micelles. | Miyo.78A174 |
| 12.9.2 | H ₂ O (pH 8.4) | $(1.7 \pm 0.2) \times 10^9$ | | 25 | A'd-20 | S = MB, A' = trypto- phan. k derived using $\beta_{A'}$ = ? and k_d = $5.0 \times 10^5 \text{ s}^{-1} [I.I]$. | Usui78F061 |
| 12.9.3 | H ₂ O (pH 7.0) | $(2.2 \pm 0.3) \times 10^9$ | | 25 | A'd-20 | S = MB, A' = diphenyl- oxazole. k derived using β_A = ? and k_d = $5.0 \times 10^5 \text{ s}^{-1} [I.I]$. A' solubilized in DTAC micelles. | Usui78F061 |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---|---|--|---------------------------------------|----------|--------|---|-------------|
| 12.9.4 | H ₂ O (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 = $5.0 \times 10^5 \text{ s}^{-1}$ [1.1]. A' solubilized in DTAC micelles. | Usui78F061 |
| 12.9.5 | H ₂ O | 2.08×10^9 | | rt | P"a-23 | S = A' = 1-anthracene sulfonate, A" = KI, P" = I_3 k derived using k_d = 5.0×10^5 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). | Hast72F515 |
| 12.9.7 | МеОН | 2.3×10^8 *1.6 × 10 ⁸ | | rt | A'd-23 | S = Py, A' = DPBF. k derived using k_d = 1.4×10^5 (*1.0 × 10 ⁵) s ⁻¹ [1.3]. | Miyo.78A174 |
| 12.9.8 | H ₂ O/MeOF (4:1) v:v | 11.33×10° (est) | | rt | P"a-23 | S = A' = 1-anthracene sulfonate, A" = KI, $P'' = I_3$. k estimated using $k_d = 4.0 \times 10^5 \text{ s}^{-1}$ (calc). | Gupt.78F183 |
| 12.9.9 | H ₂ O/MeOH (3:2) v:v | H 1.13×10° (est) | | rt | P"a-23 | S = A' = 1-anthracene sulfonate, A" = KI, P" = I_3 k estimated using $k_d = 3.2 \times 10^5 \text{ s}^{-1}$ (calc). | Gupt.78F183 |
| 12.9.10 | H ₂ O/MeOF (2:3) v:v | I 5.2×10 ⁸ (est) | | rt | P"a-23 | S = A' = 1-anthracene sulfonate, A" = KI, P" = I_3 - k estimated using $k_d = 2.5 \times 10^5 \text{ s}^{-1}$ (calc). | Gupt.78F183 |
| 12.9.11 | H ₂ O/MeOH (1:4) v:v | I 3.0×10 ⁸ (est) | | rt | P"a-23 | S = A' = 1-anthracene sulfonate, A" = KI, P" = I_3 . k estimated using $k_d = 1.9 \times 10^5 \text{ s}^{-1}$ (calc). | Gupt.78F183 |
| 12.10 superoxide ion [(CH ₃) ₄ NJO ₂ | CH ₃ CN | $(7 \pm 6) \times 10^9$ *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 × 10 ⁴ (*2.55 × 10 ⁴) s^{-1} [1.17]. | Guir.76E072 |
| 12.10.1 | Me ₂ SO | 1.6×10^{9} (est) | $(3.3 \pm 0.5) \times 10^{-5}$ | rt | A'd-16 | S = RB, A' = DPBF. k estimated using $k_d = 5.2 \times 10^4 \text{ s}^{-1}$ [1(a).1]. | Guir.76E072 |
| 12.11 superoxide ion ([CH ₃ (CH ₂) ₂ CH ₂] ₄ N | C ₆ H ₃ Br I)O ₂ /CH ₃ CN (2:1) v:v | $(3.6 \pm 0.1) \times 10^7$ N (est) | | rt | A'd-23 | S = A' = Rub. k estimated using $k_d = 3.07 \times 10^4 \text{ s}^{-1}$ (calc) and $k_{A'} = 4 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. Showed $k_q >> k_r$. | Rose75F578 |

^aThe 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 | $\beta (k_d/k)$ /mol dm ⁻³ | <i>t</i> /°℃ | Method | Comments | Ref. |
|------|--|--|--|---------------------------------------|-----------------|--------------|--|-------------|
| | | | | less k , (chemical reaction) | | | | |
| 3.1 | $\operatorname{or} \kappa_{q} (\operatorname{quenchin})$ | | | the rate constant for s | | | | W . 7(E105 |
| 13.1 | (CH ₃) ₂ C=NOH | МеОН | $k_{\rm r} \le 1.0 \times 10^4$ *1.2 × 10 ⁴ | | rt | Pa | S = RB, A' = 2M2B, P = acetophenone. Measured $(k_t/k_t^{A'})$ = 7.7×10^{-3} . k_t derived using $k_t^{A'}$ = 1.3×10^6 (*1.5 × 10 ⁶) dm ³ mol ⁻¹ s ⁻¹ [A3.1]. | Wams.76F197 |
| 13.2 | benzophenone oximate anion $(C_6H_5)_2C = NO^-$ | МеОН | $k_r = 3.4 \times 10^5$ *3.9 × 10 ⁵ | | rt | A'd-17 Pa | The first section of the first section $A' = 2M2B$, $A' $ | Wams.76F197 |
| 13.3 | benzophenone oxime $(C_6H_5)_2C=NOH$ | МеОН | $k_r = 7.7 \times 10^4$ *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 $(C_6H_3)_2C = NOCH_3$ | 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 × 10 ⁶ (*1.5 × 10 ⁶) dm ³ mol ⁻¹ s ⁻¹ [A3.1]. | Wams.76F197 |
| | | | | COMPOUNDS 13.5 | and 13.6 | : | ~ (). | |
| | | | | 5 N 2 | | | | · |
| 13.5 | 4,5,5-trimethyl- Δ^1 - pyrroline- N -oxide $[R_4 = R_5 = R_5 = -1]$ | • | 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 $[R_2 = R_4 = R_4 = -]$ | , | 2.1×10^7 | | rt | A'd-16 | S = MB, A' = DPBF. k derived using k_d (unreported). | Chin75F653 |
| 13.7 | 2-methyl-2-nitroso- propane (CH ₃) ₃ CNO | | 9.3 × 10 ⁹ (est) | | rt | A'd-32 | 1 O ₂ * from (PhO) ₃ PO ₃ decomp., A' = Rub. k estimated using $k_{A'}$ = 4.0 × 10 ⁷ dm ³ mol ⁻¹ s ⁻¹ and k_{d} = 1.1 × 10 ⁴ s ⁻¹ [1(a).10]. | Sing.76F900 |
| 13.8 | trans-1,4-dichloro- 1,4-dinitrosocyclo- hexane | CH ₂ Cl ₂ /MeOH (11:5) v:v | 5.3 × 10° (est) | | rt | A'd-32 | $^{1}O_{2}$ * from (PhO) ₃ PO ₃ decomp., A' = Rub. k estimated using $k_{A'}$ = 4.0×10^{7} dm ³ mol ⁻¹ s ⁻¹ and k_{d} = 1.9×10^{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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------|---|--|--|---------------------------------------|----------|--------|--|-------------|
| 13.9 | cis-1,4-dichloro- 1,4-dinitrosocyclo- hexane | CH ₂ Cl ₂ /MeOH (11:5) v:v | ` ' | | rt | | S = chlorophyll-a, A' = DPBF. k estimated using $k_{A'} = 8 \times 10^8 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [5.36.9] and $k_{d} = 2.1 \times 10^4 \text{ s}^{-1} [1(a).9]$. Assumed that quenching is due to 13.9 in equilibrium with 13.10. | Sing.76F900 |
| 13.9. | , | CH ₂ Cl ₂ /MeOH (11:5) v:v | 1.2 × 10 ¹⁰ (est) | | rt | A'd-32 | $^{1}O_{2}^{*}$ from (PhO) ₃ PO ₃ decomp., $A' = \text{Rub. } k$ estimated using $k_{A'} =$ $4.0 \times 10^{7} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1}$ and $k_{d} = 2.1 \times 10^{4} \text{ s}^{-1}$ {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 ₂ Cl ₃ /MeOH (11:5) v:v | 8.0 × 10 ⁷ (est) | | rt | A'd-32 | | Sing.76F900 |
| 13.11 | C, C, C, C | CH ₂ Cl ₂ /MeOH (11:5) v:v | < 2 × 10 ⁶ (est) | | rt | A'd-32 | $^{1}O_{2}^{*}$ from (PhO) ₃ PO ₃ decomp., A' = Rub. k estimated using $k_{A'}$ = 4.0×10^{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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|--|---|---|---------------------------------------|----------|-----------------------|--|-------------|
| | | | erall rate constant unlike is specified; k_d is the | | | | | |
| 14.1 | benzoquinone | EtOH | 3.4×10^{7} (est) | | rt | | S = RB, A' = chloro- phyll-a. k estimated using $k_d = 1 \times 10^5$ s ⁻¹ (calc). | Koka.78F404 |
| 14.1.1 | l | C ₆ H ₆ /Ete (2:1) v:v | OH 1.62 × 10 ⁷ (est) | | rt | A'd-19 | S = RB, A' = chloro- phyll-a. k estimated using $k_d = 1 \times 10^5$ | Koka.78F404 |
| 14.2 | ascorbic acid | МеОН | 8.3 × 10 ⁶ | 1.2×10^{-2} | 20 | Od-15 | s ⁻¹ (calc). S = RB. k derived using $k_d = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. $E_a = 63 \text{ kJ mol}^{-1}$. | Koch68F288 |
| 14.3 | α-tocopheryl acetate H ₃ C CH ₃ C | C₅H₅N н₃ сн₃ сн₂сн₂сн ъ с | < 1.6 × 10 ⁶ | | rt | A'd-23 | S = A' = Rub. k derived using $k_{A'}$ = $4 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ and $k_d = *6.0 \times 10^4 \text{ s}^{-1}$ [1.29.1]. | Fahr74R112 |
| 4.4 | methyl stearate CH ₃ (CH ₂) ₁₆ COOC | C ₅ H ₅ N H. | $k_{\rm r} \leqslant 5 \times 10^4$ | | rt | Ad-17 A'd | S = protoporphyrin, A' = cholesterol. No measurable effect. | Dole74R115 |
| 4.5 | methyl oleate $CH_3(CH_2)_7CH = C$ | EtOH | 1.3 × 10 ⁵ | 6.3×10^{-1} | 20 | Pa-15 | S = MB, P = methyloleatemonohydroperoxide. k derived using $k_d = *7.9 \times 10^4$ s ⁻¹ [1.10.3]. | Tera.77F378 |
| 4.5.1 | | C₅H₅N | $k_{\rm r}=7.3\times10^6$ | v | rt | Ad-17 A'd (sep) | S = protoporphyrin, A' = cholesterol. Measured $(k_r/k_r^{A'})$ = 1.1. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm³ mol ⁻¹ s ⁻¹ [14.9]. | Dole74R115 |
| 4.5.2 | | C ₅ H ₅ N | $k_{\rm r}=9.2\times10^4$ | | rt | Ad-17 A'd (sep) | S = protoporphyrin, A' = cholesterol. Measured $(k_r/k_r^{A'})$ = 1.4. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm³ mol ⁻¹ s ⁻¹ [14.9]. | Dole74R115 |
| 4.6 | methyl linoleate $CH_3(CH_2)_4CH = C$ | EtOH HCH ₂ CH=0 | 2.2×10^{5} CH(CH ₂),COOCH ₃ | 3.6×10^{-1} | 20 | Pa-15 | S = MB, P = methyl- linoleatemonohydro- peroxide. k derived using $k_d = *7.9 \times 10^4$ | Tera.77F378 |
| 14.6.1 | | C,H,N | $k_{\rm r}=1.2\times10^{\rm 5}$ | , | rt | Ad-17 A'd (sep) | s ⁻¹ [1.10.3]. S = protoporphyrin, A' = cholesterol. Measured $(k_r/k_r^{A'})$ = 1.9. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm³ mol ⁻¹ s ⁻¹ [14.9]. | Dole74R115 |

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

| No. Substrate (A | A) Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------------------------|--|---|---------------------------------------|-------------------------------|------------------------------------|--|-------------------|
| 14.6.2 | C₃H₃N | $k_{\rm r}=1.3\times10^5$ | | rt | Ad-17 A'd (sep) | S = protoporphyrin, A' = cholesterol. Measured (k_r/k_r^A) = 2.0 ± 0.2 . k_r derived using $k_r^A = k_{A'} =$ 6.6×10^4 dm ³ mol ⁻¹ s ⁻¹ [A3.19]. | Dole74F115 |
| 14.7 methyl line | olenate EtOH | For more relative re 2.9×10^5 | tes see $4.25.3$ $2.7 	imes 10^{-1}$ | 2, 4.27.2, 4 20 | .28.6. Pa−15 | S _ MD D _ mothul | Tera.77F378 |
| • | $CH = CH)_3CH_2(CH_2)_6$ | | 2.7 × 10 | 20 | Fa-13 | S = MB, P = methyllinolenatemonohydroperoxide. k derived using $k_d = *7.9 \times 10^4$ s ⁻¹ [1.10.3]. | 1 eta. // F 3 / 6 |
| 14.7.1 | C,H,N | $k_{\rm r}=1.9\times10^{\rm 5}$ | | rt | Ad-17 A'd (sep) | S = protoporphyrin, A' = cholesterol. Measured $(k_r/k_r^{\Lambda'})$ = 2.9. k_r derived using $k_r^{\Lambda'} = k_{\Lambda'} = 6.6 \times 10^4$ dm³ mol ⁻¹ s ⁻¹ [14.9]. | Dole74R115 |
| 14.7.2 | C ₅ H ₅ N | $k_{\rm r}=1.8\times10^5$ | | rt | Ad-17 A'd | | Dole74R115 |
| 14.7.3 | C₃H₅N | 1.6×10^5 | | rt | A'd-23 | S = A' = Rub. k derived using k_A = 4.0×10^7 dm ³ mol ⁻¹ s ⁻¹ and k_d = 6.0×10^4 s ⁻¹ [1.29.1]. | Dole74R115 |
| | chidonate C_5H_5N $(CH = CHCH_2)_4CH_2$ | $k_{\rm r} = 2.2 \times 10^{\rm 5}$ ${\rm CH_2COOCH_3}$ | | rt | Ad-17 A'd (sep) | S = protoporphyrin, A' = cholesterol. Measured $(k_r/k_r^{A'}) =$ | Dole74R115 |
| | | | | | | 3.4. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm ³ mol ⁻¹ s ⁻¹ [14.9]. | |
| 14.8.1 | C₃H₃N | $k_{\rm r}=2.9\times10^{\rm 5}$ | | rt | Ad-17 A'd | S = protoporphyrin, A' = cholesterol. Measured (k_r/k_r^A) = 4.4. k_r derived using $k_r^{A'} = k_{A'} = 6.6 \times 10^4$ dm³ mol ⁻¹ s ⁻¹ [14.9]. | Dole74R115 |
| 14.9 cholesterol | C ₃ H ₅ N | 6.6 × 10 ⁴ | 8.94 × 10 ⁻¹ | 20 | Od-15 | S = hematoporphyrin. k derived using $k_d = *5.9 \times 10^4$ s ⁻¹ [1.29.1]. | Sche57F008 |
| 14.10 cholestery benzoate | yl C ₆ H ₆ /C ₅ H ₅ N (10:1) v:v | For more relative re 1.1×10^4 (est) | stes see 14.4, 1 3.98 | 4.5.1–2, 1 ⁴ 20 | 4.6.1–2, 14. [°] Od–15 | 7.1-2, 14.8, 14.8.1. S = hematoporphyrin. k estimated using $k_d = 4.2 \times 10^4 \text{ s}^{-1} \text{ (calc)}.$ | Sche57F008 |
| a | CH ₃ | СН ₃ | | | | | |

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

| No. Substrate (A) | Solvent | k /dm³ mol-¹ s-1 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--|---|----------------------------------|---------------------------------------|----------|--------|--|-------------|
| 14.11 ergosterol | C ₅ H ₅ N | 1.3 × 10 ⁷ | 4.5 × 10 ⁻³ | 20 | Od-15 | S = hematoporphyrin. k derived using $k_d = *5.9 \times 10^4$ s^{-1} [1.29.1]. | Sche57F008 |
| 14.12 pregnenolone | C ₅ H ₅ N | 3.5 × 10 ⁴ | 1.71 | 20 | Od-15 | S = hematoporphyrin. k derived using $k_d = *5.9 \times 10^4$ s^{-1} [1.29.1]. | Sche.58F002 |
| 14.12.1 | C ₆ H ₆ /C ₅ H ₅ N (3:2) v:v | 2.7×10^4 (est) | 1.79 | 20, | Od-15 | k estimated using $k_d =$ | Sche58F002 |
| 14.12.2 | C ₆ H ₆ /C ₅ H ₅ N (5:2) v:v | 0.5×10^4 (est) | 1.82 | 20 | Od-15 | $4.8 \times 10^4 \mathrm{s}^{-1}$ (calc). S = hematoporphyrin. k estimated using $k_{\rm d} = 4.6 \times 10^4 \mathrm{s}^{-1}$ (calc). | Sche57F008 |
| 14.13 stigmasteryl acetate | C ₆ H ₆ /C ₅ H ₅ N (10:1) v:v | CH ₃ | 4.06 | 20 | Od-15 | | Sche57F008 |
| 14.14 sitosteryl acetate | C ₆ H ₆ /C ₅ H ₅ N (10:1) v:v | | 6.50 | 20 | Od-15 | S = hematoporphyrin. k estimated using k_d = $4.2 \times 10^4 \text{ s}^{-1}$ (calc). | Sche57F008 |
| 14.15 16-dehydropreg nenolone-3-ace | | 9.0 × 10 ³ V (est) | 4.65 | 20 | Od-15 | S = hematoporphyrin. k estimated using k_d = $4.2 \times 10^4 \text{ s}^{-1}$ (calc). | Sche57F008 |
| 14.16 7-dehydroandro sterone-3-aceta | | 6.6×10^{3} (est) | 6.34 | 20 | Od-15 | S = hematoporphyrin. k estimated using k_d = $4.2 \times 10^4 \text{s}^{-1}$ (calc). | Sche57F008 |

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

| No. S | Substrate (A) | Solvent | k /dm³ mo1-1 s-1 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|---|-------------------|---|---------------------------------------|----------|--------|--|-------------|
| 14.17 | 5'-oxo-4'-vinyl -4-ethyl-3',3,5-tri- methyl-1',5'-di- hydro-(2.2')-di- pyrromethene | МеОН | 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 |
| | CH ₂ =CH | CH ₃ | н | | | | | |
| |) М—н н | CH ₃ | | | | | | |
| 14.17.1 | | MeOH | $k_{\rm r}=8.5\times10^8$ | | 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 × 10° | | rt | Ad-15 | | Ligh.79F104 |
| 14.17.3 | | CHCl ₃ | $k_{\rm r} = 1.9 \times 10^9$ *1.1 × 10 ⁹ | * | rt | Ad-15 | $S = RBCE$. k_r derived | Ligh.79F104 |
| 14.18 | 5'-oxo-3',4',4- triethyl-3,5-di- methyl-1',5'- dihydro-(2.2')-di- pyrromethene | МеОН | 1.9 × 10 ⁹ | | rt | Ad-15 | using $\phi_{\rm isc} = 0.36$. S = RB. k derived using $k_{\rm d} = *1.0 \times 10^5$ s^{-1} [1.3.6]. | Ligh.79F104 |
| | CH ₂ CH ₂ N-H H-N | CH ₃ | | | | | | |
| 14.18.1 | | МеОН | $k_{\rm r}=9.9\times10^8$ | | 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 × 10° | | rt | Ad-15 | | Ligh.79F104 |
| 14.18.3 | | CHCl ₃ | $k_{\rm r} = 3.2 \times 10^9$ *1.9 × 10 ⁹ | | rt | Ad-15 | | Ligh.79F104 |
| 14.19 | 5'-oxo-3'-ethyl- 4',3,5-trimethyl- 1,5'-dihydro- (2.2')-dipyrro- methene | МеОН | 7.9×10^8 | | rt | Ad-15 | | Ligh.79F104 |
| | CH ₂ CH ₃ | СН ₃ | | | | | | |
| 14.19.1 | | МеОН | $k_{\rm r}=4.3\times10^8$ | | 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 × 10° | | 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 |
| 14.19.3 | | CHCl ₃ | $k_{\rm r} = 1.6 \times 10^9$ *9.3 × 10 ⁸ | | rt | Ad-15 | $S = RBCE$. k_r derived | Ligh.79F104 |
| 14.20 | 5'-oxo-4',4,5-tri- methyl-3'-ethyl- 1,5'-dihydro- (2.2')-dipyrro- methene | МеОН | 1.6 × 10° | | rt | Ad-15 | using $\phi_{\rm isc} = 0.36$. S = RB. k derived using $k_{\rm d} = *1.0 \times 10^5$ s ⁻¹ [1.3.6]. | Ligh.79F104 |
| | CH ₂ CH ₃ | сн. | | | | | | |
| 14.20.1 | - | МеОН | $k_{\rm r}=6.2\times10^8$ | | 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 /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--|---------------------------------------|---|---------------------------------------|----------|--------|--|-------------|
| 14.20.2 | CHCl ₃ | 2.5 × 10 ⁹ *1.5 × 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 |
| 14.20.3 | CHCl ₃ | $k_{\rm r} = 1.7 \times 10^9$ *1.0 × 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 | МеОН | 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 |
| CH ₃ CH ₂ -N-H H- | N CH ₃ | | | | | | |
| 4.21.1 | МеОН | $k_{\rm r}=2.1\times10^8$ | | rt | Ad-15 | $S = RB. k_r derived$ | Ligh.79F104 |
| 14.21.2 | CHCl ₃ | 1.5×10^9 *9.0 × 10 ⁸ | | rt | Ad-15 | using $\phi_{isc} = 0.76$. S = RBCE. k derived using $k_d = 1.67 \times 10^4$ (*1.0 × 10 ⁴) s ⁻¹ [1.5]. | Ligh.79F104 |
| 14.21.3 | CHCl ₃ | $k_{\rm r} = 8.0 \times 10^8$ *4.8 × 10 ⁸ | | rt | Ad-15 | $S = RBCE$. k_r derived using $\phi_{isc} = 0.36$. | Ligh.79F104 |
| 4.22 5'-oxo-4-ethyl- 3,5-dimethyl-1, 5'-dihydro-(2.2')- dipyrromethene | МеОН | 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 |
| N-H H-N CH ₃ | s -CH ₂ CH ₃ | | | | | | |
| 14.22.1 | МеОН | $k_{\rm r}=7.0\times10^7$ | | rt | Ad-15 | | Ligh.79F104 |
| 14.22.2 | CHCl ₃ | 4.4×10^9 *2.6 × 10 ⁹ | | rt | Ad-15 | using $\phi_{\rm isc} = 0.76$. $S = RBCE$. k derived using $k_{\rm d} = 1.67 \times 10^4$ | Ligh.79F104 |
| 14.22.3 | CHCl ₃ | $k_{\rm r} = 3.0 \times 10^9$ *1.8 × 10 ⁹ | | rt | Ad-15 | (*1.0 × 10 ⁴) s ⁻¹ [1.5]. 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. S | Substrate (A) | Solvent | $\frac{k}{\text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1}}$ | $\beta (k_d/k)$ /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 $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ [1.8.3]. | Kras79A010 |
| | CH ₃ CH ₃ N N N N CH ₂ CH ₃ CH ₂ CH ₃ | CH2 CH3 CH3 | CH ₃ phytyl = −CH ₂ CH= C (CH ₂ CH ₂ C | CH3 L L L2CH-)3 CH3 | | | | |
| 14.23.1 | | CCl ₄ | $k_{\rm r} = (4.0 \pm 2.8) \times 10^6$ | | rt | Ad-27 | $S = ? k_r \text{ derived}$ 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 | | Koka.78F404 |
| 14.23.3 | | C ₆ H ₆ /EtC (2:1) v:v | $0H 1.2 \times 10^7$ (est) | | rt | Ad-19 | S = RB, A' = Car. k estimated using k_d = 1×10^5 s ⁻¹ (calc). | Koka.78F404 |
| 14.24 | protochlorophyll ^{CH2} | CCl ₄ | $ < 1 \times 10^8 $ (est) | | rt | Ld-13 | $S = ? k$ estimated using $k_d = 3.6 \times 10^1 \text{ s}^{-1}[1.8.3]$. Analysis complicated by a protopheophytin impurity. | Kras79A010 |
| | CH2 | | | | | | | |
| 14.24.1 | | CCl ₄ | $k_{\rm r} < 1 \times 10^6$ (est) | | rt | Ad-27 | $S = ? k_r \text{ estimated}$ using $k_A = 1.0 \times 10^8$ | Kras79A010 |
| 14.25 | bacterio- chlorophyll-a | CCl ₄ | $(1.0 \pm 0.3) \times 10^9$ | | rt | Ld-13 | dm ³ mol ⁻¹ s ⁻¹ [14.24]. S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ [1.8.3]. | Kras79A010 |
| | 0 C-CH ₃ CH ₃ N N N N N N N N N N N N N N N N N N N | CH ₂ CH3 | | | | | | |

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

| t Method Comments R | Ref. |
|---|------------|
| rt Ld-13 S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ [1.8.3]. | Kras79A010 |
| | |
| | |
| | |
| rt Ad-27 S = $? k_r$ derived K | Kras79A01 |
| using $k_A = 2.0 \times 10^7$ dm ³ mol ⁻¹ s ⁻¹ [14.26]. | KIAS/9AUI |
| rt Ld-13 S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ [1.8.3]. | Kras79A01 |
| | |
| | |
| rt Ad-27 S = ? k_r derived K using $k_A = 2.0 \times 10^8$ dm³ mol ⁻¹ s ⁻¹ [14.27]. | Kras79A01 |
| rt Ld-13 S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ [1.8.3]. | Kras79A01 |
| | |
| $k_{\rm d} = 3.6 \times 10^1 \rm s^{-1}$ | , 1 |

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

| No. 5 | Substrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_{d}/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|--|---|--|---|----------|--------|---|-------------|
| 14.29 | tetraphenylbact- eriochlorin-trans | CCI ₄ | $(1.0 \pm 0.3) \times 10^8$ | | rt | Ld-13 | S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ [1.8.3]. | Kras79A010 |
| | I C ₆ H ₅ | | | | | | | |
| 14.29.1 | | CCl ₄ | $k_{\rm r}=2\times10^5$ | | rt | Ad-27 | $S = ? k_r \text{ derived}$ using $k_A = 1.0 \times 10^8$ | Kras79A010 |
| 14.30 | tetraphenyl- porphine | CCl ₄ | $(1.0 \pm 0.3) \times 10^6$ | | rt | Ld-13 | dm ³ mol ⁻¹ s ⁻¹ [14.29]. S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ [1.8.3]. | Kras79A010 |
| | CeH5 | _ c _е н _я | | | | | | |
| 14.30.1 | | CCl ₄ | $k_{\rm r} = (3.0 \pm 2.1) \times 10^2$ | | rt | Ad-27 | $S = ? k_r \text{ derived}$ using $k_A = 1.0 \times 10^6$ | Kras79A010 |
| 14.31 | mesoporphyrin- IX-dimethyl ester | CCl ₄ | $(2.5 \pm 0.8) \times 10^6$ | | rt | Ld-13 | dm ³ mol ⁻¹ s ⁻¹ [14.30]. S = ? k derived using $k_d = 3.6 \times 10^1 \text{ s}^{-1}$ | Kras79A010 |
| 14.32 | bilirubin | D ₂ O (pD 7) | $k_{\rm r} = (1.5 \pm 0.4) \times 10^7 +9.3 \times 10^6$ | | rt | Ad-35 | [1.8.3]. ${}^{1}O_{2}^{*}$ from Nd-YAG CW laser (1065 nm). k_{r} derived using $k_{d} =$ 5.0×10^{4} (*3.1 × 10 ⁴) s^{-1} [1.2.3]. | Math74F103 |
| | H ₃ C CH ₂ =CH H ₃ C CH ₂ HOOC - C | CH ₂ N H ₂ CH ₂ CH ₂ COO | CH CH=CH ₂ | | | | | |
| 14.32.1 | | D ₂ O (pD 10) | $k_{\rm r} = (3.0 \pm 0.7) \times 10^9$ *1.9 × 10 ⁹ | | rt | Ad-35 | $^{1}\text{O}_{2}^{*}$ from Nd-YAG CW laser (1065 nm). k_{r} derived using $k_{\text{d}} = 5.0 \times 10^{4} (*3.1 \times 10^{4})$ s ⁻¹ [1.2.3]. | Math74F103 |
| | | | | | | | | |
| | | | | | | | | |
| 14.32.2 | | МеОН | 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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|--|---|---------------------------------------|----------|--------------|---|-------------|
| 14.32.3 | МеОН | $k_{\rm r}=2.0\times10^8$ | | 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° | $(7.7 \pm 3.0) \times 10^{-6}$ | 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 | CHCI, | $k_{\rm r} = 4.3 \times 10^8$ *2.7 × 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 × 10 ⁷ (*3.0 × 10 ⁷) dm ³ mol ⁻¹ s ⁻¹ [2.35.2]. | Foot.75R071 |
| 14.32.7 | CHCl ₃ | $k_{\rm r} = 2.1 \times 10^8$ *1.9 × 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 × 10 ⁸ (*6.3 × 10 ⁸) dm ³ mol ⁻¹ s ⁻¹ [5.36.85]. | Foot.75R071 |
| 14.32.8 | CHCl ₃ | 2.8×10^9 *1.7 × 10° | | rt | Ad-15 | | Ligh.79F104 |
| 14.32.9 | CHCl ₃ | $k_{\rm r} = 3.8 \times 10^8$ *2.3 × 10 ⁸ | | rt | Ad-15 | | Ligh.79F104 |
| 14.32.10 | CCl₄ | $k_{\rm r} = (1.7 \pm 0.3) \times 10^8 \times 10^8 = (2.3 \pm 1.0) \times 10^9$ | | 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 | $k_{\rm r}=1.7\times10^8$ | | rt | A'd-17 Ad | S = A' = Rub. Measured $(k_r/k_r^{A'}) = 4 \pm 1$. k_r derived using $k_r^{A'} = 4.2 \times 10^7 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [3.63.1]. | Stev.76R011 |
| 14.32.12 | CCl ₂ F- CClF ₂ | $k_{\rm r} = (1.0 \pm 0.4) \times 10^7$ | | rt | Ad-36 | $^{1}O_{2}*$ from Nd-YAG CW laser (1065 nm). k_{r} derived using $k_{O2} = 2.7 \times 10^{3} \text{ dm}^{3} \text{ mol}^{-1} \text{ s}^{-1} [15.1.4].$ | Math74F103 |
| 14.32.13 | CCl ₂ F- CClF ₂ | $k_{\rm r} = (1.0 \pm 0.2) \times 10^8$ | | rt | Ad-36 | $^{1}O_{2}*$ from Nd-YAG CW laser (1065 nm). k_{r} derived using $k_{O2} = 2.7 \times 10^{3}$ dm 3 mol $^{-1}$ s $^{-1}$ [15.1.4]. Previous value by same workers [74F103] low due to overdepletion of A in solution exposed | Math.77F129 |
| 14.32.14 | C ₆ H ₆ | $k_{\rm r}=1.7\times10^8$ | | rt | A'd-17 Ad | directly to laser beam. $S = A' = Rub$. Measured $(k_r/k_r^{A'}) = 4 \pm 1$. 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 | | 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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|------------------------------|---|---|---------------------------------------|----------|--------------|--|-------------|
| 14.32.16 | CHCl ₃ /MeOH (9:1) v:v | $k_{\rm r}=2.5\times10^8$ | | rt | Ad-14 | S = RB. k_r derived using $\phi_{isc} = 0.66$ and $k_A = 1.5 \times 10^9$ dm ³ | Foot.75R071 |
| 14.33 aetiobilirubin -IVγ | CHCl ₃ | 3.0×10^{9} $*1.8 \times 10^{9}$ | | rt | Ad-15 | mol ⁻¹ s ⁻¹ [14.32.4]. 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 | $k_{\rm r} = 2.3 \times 10^9$ *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 $k_d = *1.0 \times 10^5$ $s^{-1} [1.3.6].$ | Ligh.79F104 |
| 14.33.3 | MeOH /CHCl ₃ (9:1) v:v | $k_{\rm r}=6.2\times10^8$ | | rt | Ad-15 | | Ligh.79F104 |
| 14.34 biliveridin | D ₂ O (pD 8.4) | $k_{r}(3.0 \pm 0.1) \times 10^{8}$ | | rt | Ad-35 | $^{1}O_{2}*$ from Nd-YAG CW laser (1065 nm). k_{r} derived using $k_{d} = 5.0 \times 10^{4} \text{ s}^{-1}$ and $k_{A} = 5.1 \times 10^{10}$ dm ³ mol ⁻¹ s ⁻¹ [14.34.1]. | Math.77F129 |
| 14.34.1 | D ₂ O (pD 8.4) | $(5.1 \pm 0.4) \times 10^{10}$ | | rt | A'd-16 | $^{1}O_{2}^{*}$ from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived | Math.77F129 |
| 14.34.2 | D ₂ O (pD 11.8) | $k_{\rm r} = (4.0 \pm 0.4) \times 10^8$ | | rt | Ad-35 | using $k_d = 5.0 \times 10^4 \text{ s}^{-1}$. ${}^{1}O_2^*$ from Nd-YAG CW laser (1065 nm). k_r derived using $k_d = 5.0 \times 10^4 \text{ s}^{-1}$ and $k_A = 6.0 \times 10^{10}$ dm ³ mol ⁻¹ s ⁻¹ [14.34.3]. | Math.77F129 |
| 14.34.3 | D ₂ O (pD 11.8) | $(6.0 \pm 2.0) \times 10^{10}$ | | rt | A'd-16 | $^{1}O_{2}$ * from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived using $k_{d} = 5.0 \times 10^{4} \text{ s}^{-1}$. | Math.77F129 |
| 14.34.4 | D ₂ O (pD 13.4) | $k_{\rm r} = (5.1 \pm 1.2) \times 10^8$ | | rt | Ad-35 | 1 O ₂ * from Nd-YAG laser (1065 nm). k_r derived using $k_d = 5.0 \times 10^4 \text{ s}^{-1}$ and $k_A = 1.5 \times 10^{10}$ dm ³ mol ⁻¹ s ⁻¹ [14.34.5]. | Math.77F129 |
| 14.34.5 | D ₂ O (pD 13.4) | $(1.5 \pm 0.3) \times 10^{10}$ | | rt | A'd-16 | $^{1}O_{2}$ * from Nd-YAG laser (1065 nm), A' = bilirubin. k derived using $k_{d} = 5.0 \times 10^{4} \text{ s}^{-1}$. | Math.77F129 |
| 14.34.6 | CHCI, | $k_{\rm r} \leqslant 2.9 \times 10^6$ | | rt | Ad-17 A'd | S = A' = Rub. Measured $(k_r/k_r^{A'}) \le 0.07$. k_r derived using $k_r^{A'} = 4.2 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} [3.63.1]$. | 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 = $*1.0 \times 10^4 \text{ s}^{-1} [1.5.3]$. | Stev.76R011 |

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

| No. S | Substrate (A) | Solvent | k /dm ³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---------|-------------------------------|--|---|---------------------------------------|----------|--------|---|-------------|
| 14.35 | biliveridin dimethyl ester | CCI ₂ F- CCIF ₂ | $k_{\rm r} = (6.0 \pm 0.5)$ $\times 10^5$ $c_{\rm CH_3}$ $c_{\rm H_3}$ $c_{\rm CH_2}$ $c_{\rm H_3}$ | | rt · | A'd-35 | $^{1}\text{O}_{2}$ * from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived using $k_{\text{O}_{2}} = 2.7 \times 10^{3}$ [15.1.4]. | Math.77F129 |
| 14.35. | ı | CCl ₂ F- CClF ₂ | $k_{\rm q} = (8.0 \pm 2.0) \times 10^8$ | | rt | A'd-35 | $^{1}\text{O}_{2}$ * from Nd-YAG CW laser (1065 nm), A' = bilirubin. k derived using $k_{\text{O}2} = 2.7 \times 10^{3}$ [15.1.4]. | Math.77F129 |
| 14.35.2 | | CCl ₂ F- CClF ₂ | 9 × 10 ⁸ | | rt | A'd-16 | | Math.77F129 |
| 14.36 | guanosine | H ₂ O (pH 7.1) | ≤ 1 × 10 ⁶ | | 25 | Od-19 | S = phenosafranine. No measurable effect. | Kral.78A360 |
| | HOCH2 HOCH2 OH OH | | | | | | | |
| 14.36.1 | | H ₂ O/MeOl (1:1) v:v | H <1×10 ⁷ | | rt | A'd-5 | S = MB, A' = DPBF, | Nils72F516 |
| 14.37 | adenine | H_2O (pH 7.1) | ≤ 1 × 10 ⁶ | | 25 | Od-19 | ruby laser (694 nm). S = phenosafranine. No measurable effect. | Kral.78A360 |
| | NH2 I | | | | | | | |
| 14.38 | adenosine | H ₂ O (pH 7.1) | < 1 × 10 ⁶ | | 25 | Od-19 | S = phenosafranine. No measurable effect. | Kral.78A360 |
| | HOCH2 HOCH2 H H H | | | | | | | |
| 14.39 | thymine | H ₂ O (pH 7.1) | ≤ 1 × 10 ⁶ | | 25 | Od-19 | S = phenosafranine. No measurable effect. | Kral.78A360 |
| | H ₃ C NH | | | | | | | |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-------------------|------------------------------|--|---------------------------------------|----------|--------|--|-------------|
| 14.40 cytidine | H ₂ O (pH 7.1) | ≤ 1 × 10 ⁶ | | 25 | Od-19 | S = phenosafranine. No measurable effect. | Kral.78A360 |
| NH ₂ | | | | | | | |
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TABLE 15. Rate constants for the interaction of singlet oxygen with miscellaneous substrates

| 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 re | epresents the | overall rate constant u | nless k_r (chemical react | tion ra | te constant) | | |
| or k_{q} (quenching | rate constan | nt) is specified; $k_{\rm d}$ is the | rate constant for solve | nt dea | ctivation] | • | |
| 15.1 oxygen $(^{3}\Sigma_{g})$ O ₂ | H ₂ O (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 $k_d = *4.4 \times 10^5$ s ⁻¹ [1.1.3]. | Koiz.68F287 |
| 15.1.1 | H ₂ O (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 $k_d = *4.4 \times 10^5$ s ⁻¹ [1.1.3]. | Koiz.68F287 |
| 15.1.2 | H ₂ O (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 $k_d = *4.4 \times 10^5$ s ⁻¹ [1.1.3]. | Koiz.68F287 |
| 15.1.3 | H ₂ O (pH 6.2) | 2.6 × 10 ⁴ | 6.0×10^{-2} | , | A'd-19 | S = acridine, A' = leuco fluorescein. k derived using $k_d = *4.4 \times 10^5$ | Koiz.68F287 |
| 15.1.4 | CC1 ₂ F- CC1F ₂ | $(2.7 \pm 0.3) \times 10^3$ | | rt | A'd-5 | s ⁻¹ [1.1.3]. ¹ O ₂ * from pulsed Nd-YAG laser (1065 nm), A' = DPBF. | Math74F102 |
| 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 ₃ OH | CCl₄ | $(3.0 \pm 1.0) \times 10^3$ | | rt | A'd-8 | S = MB, $A' = DPBF$, dye laser (610 nm). | Youn.76F903 |
| 15.3 ethanol CH ₃ CH ₂ OH | 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 ₃ CH ₂ I | C_6H_6 | 2×10^4 | | rt | A'd-8 | S = An, $A' = DPBF$, ruby laser (347 nm). | Wilk76F902 |
| 15.4.1 | C ₆ H ₅ Br /Me ₂ C | ≤ 10 ⁶ | | rt | A'd-23 | S = A' = Rub. No measurable effect. | Rose.76F126 |
| • , | (2:1) v:v | | | | | measurable effect. | |
| 15.4.2 | C ₆ H ₅ Br /MeO | ≤ 10 ⁶ H | | rt | A'd-23 | S = A' = Rub. No measurable effect. | Rose.76F126 |
| 2-propanol CH ₃ CH(OH)CH ₃ | (2:1) v:v CCl ₄ | $(1.7 \pm 0.9) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, | Youn.76F903 |
| 15.6 l-butanol CH ₃ (CH ₂) ₂ CH ₂ OH | CCl ₄ | $(2.4 \pm 0.6) \times 10^3$ | | rt | A'd-8 | dye laser (610 nm). S = MB, A' = DPBF, | Youn76F903 |
| 15.7 2-methyl-2- propanol $(CH_3)_3COH$ | CCl ₄ | $(1.8 \pm 1.5) \times 10^3$ | | rt | A'd-8 | dye laser (610 nm). S = MB, A' = DPBF, dye laser (610 nm). | Youn76F903 |
| 15.8 heptane $CH_3(CH_2)_5CH_3$ | CCl ₄ /Met (96:4) v:v | OH (4 \pm 2) \times 10 ² | | rt | A'd-8 | S = MB, A' = DPBF, | Bort77F162 |
| 5.9 3-methylheptane | CCl ₄ /Met (96:4) v:v | OH (5.5 \pm 2.5) \times 10 ² | | rt | A'd-8 | ruby laser (694 nm). S = MB, A' = DPBF, ruby laser (694 nm). | Bort77F162 |
| CH ₃ (CH ₂) ₃ CH(CH ₃ | | | | | | . , | • |
| 15.10 4-methylheptane | (96:4) v:v | | | rt | A'd-8 | S = MB, $A' = DPBF$, ruby laser (694 nm). | Bort77F162 |
| CH ₃ (CH ₂) ₂ CH(CH tetrahydrofuran | I ₃)(CH ₂) ₂ CH CCl ₄ | $(1.9 \pm 1.1) \times 10^3$ | | rt | A'd-8 | S = MB, A' = DPBF, | Youn.76F903 |
| , | | | | | | dye laser (610 nm). | 22 |

COMPOUNDS 15.12 - 15.18:



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

| No. Subs | strate (A) | Solvent | k /dm³ mol ⁻¹ s ⁻¹ | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|-----------|--|---------------------------------|--|---------------------------------------|----------|--------------|---|------------|
| 15.12 2,3 | 3-dihydropyran | (Me) ₂ CO | $k_r = 7.2 \times 10^4$ *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 × 10 ⁵ (*1.8 × 10 ⁵) dm ³ mol ⁻¹ | Bart70F733 |
| dil | methyl-2,3- hydropyran-2- t $k_2 = -T$, $R_4 = -C$ | CH ₃ CN ₃ | $k_{\rm r} = 6.7 \times 10^4$ (est) | | rt | Ad-17 A'd | s ⁻¹ [2.55.1]. S = MB, A' = 4-methyl-2,3-dihydropyran. Measured $(k_r^{A'}/k_r)$ = 1.067 ± 0.001. k_r estimated using $k_r^{A'}$ = $k_r(2,3-\text{dihydropyran})$ = 7.2 × 10 ⁴ dm ³ mol ⁻¹ s ⁻¹ [15.12]. | Frim77F645 |
| 15.13.1 | | C ₆ H ₆ | $k_{\rm r} = 7.3 \times 10^4$ (est) | | rt | Ad-17 A'd | | Frim77F645 |
| dih | methyl-2,3- hydropyran-3- t $_{3} = -T$, $R_{4} = -C$ | CH3CN | $k_{\rm r} = 8.3 \times 10^4$ (est) | | rt | Ad-17 A'd | | Frim77F645 |
| 15.14.1 | | C ₆ H ₆ | $k_{\rm r} = 7.9 \times 10^4 $ (est) | | rt | Ad-17 A'd | S [13.12]. S = TPP, A' = 4-methyl-2,3-dihydropyran. Measured $(k_r^{A'}/k_r) = 0.908 \pm 0.006$. k_r estimated using $k_r^{A'} = k_r(2,3-\text{dihydropyran}) = 7.2 \times 10^4 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [15.12]. | Frim77F645 |
| dih | methyl-2,3- hydropyran-4- d $_4 = -D$, $R_4 = -C$ | CH ₃ CN | $k_{\rm r} = 4.0 \times 10^4$ (est) | | rt | ? | S = MB, A' = 4-methyl- 2,3-dihydropyran. Measured $(k_r^{A'}/k_r)$ = 1.787 ± 0.050. k_r estimated using $k_r^{A'} = k_r(2,3-\text{dihydro-} \text{pyran}) = 7.2 \times 10^4 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [15.12]. | Frim77F645 |
| 15.15.1 | | C ₆ H ₆ | $k_{\rm 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 $k_r^{A'}$ = $k_r(2,3-\text{dihydropyran})$ = 7.2 × 10 ⁴ dm ³ mol ⁻¹ s ⁻¹ [15.12]. | Frim77F645 |
| dih | methyl-2,3- nydropyran-4- t $_4 = -T$, $R_4 = -Cl$ | CH ₃ CN | $k_{\rm r} = 5.9 \times 10^4$ (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 $k_r^{A'}$ = $k_r(2,3-\text{dihydropyran})$ = $7.2 \times 10^4 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [15.12]. | Frim77F645 |

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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|---|---|--|---------------------------------------|----------|--------------|---|-------------|
| 15.16.1 | C ₆ H ₆ | $k_{\rm r} = 5.4 \times 10^4$ (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 $k_r^{A'}$ = $k_r(2,3-\text{dihydropyran})$ = $7.2 \times 10^4 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [15.12]. | Frim77F645 |
| 15.17 4,4-dimethyl-2,3- dihydropyran-2- t [$R_2 = -T$, $R_4 = R_4 = -CH_3$] | CH₃CN | $k_{\rm r} = 7.2 \times 10^4$ (est) | | rt | Ad-17 A'd | S = MB, A' = 4,4-di- methyl-2,3-dihydropyran. Measured (k_r^{Λ}/k_r) = 1.001 \pm 0.015. k_r estimated using $k_r^{\Lambda'}$ = k_r (2,3-dihydropyran) = 7.2 \times 10 ⁴ dm ³ mol ⁻¹ s ⁻¹ [15.12]. | Frim77F645 |
| 15.17.1 | C ₆ H ₆ | $k_{\rm r} = 7.2 \times 10^4$ (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 $k_r^{A'}$ = $k_r(2,3-\text{dihydropyran})$ = 7.2 × 10 ⁴ dm ³ mol ⁻¹ s ⁻¹ [15.12]. | Frim77F645 |
| 15.18 4,4-dimethyl-2,3- dihydropyran-3- t [R ₃ = -T, R ₄ = R ₄ = -CH ₃] | CH ₃ CN | $k_{\rm r} = 8.0 \times 10^4$ (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 $k_r^{A'}$ = $k_r(2,3-\text{dihydropyran})$ = $7.2 \times 10^4 \text{ dm}^3 \text{ mol}^{-1}$ | Frim77F645 |
| 15.18.1 | C ₆ H ₆ | $k_{\rm r} = 8.0 \times 10^4$ (est) | | rt | Ad-17 A'd | s ⁻¹ [15.12]. 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 | Frim77F645 |
| 15.19 dioxane | CCl₄ | $(7.0 \pm 15) \times 10^2$ | | rt | A'd-8 | s ⁻¹ [15.12]. S = MB, A' = DPBF, dye laser (610 nm). | Youn.76F903 |
| 15.20 complex diketone-VIII | CH ₂ Cl ₂ C(CH ₂) ₃ C(CH ₂) ₃ | 2.3 × 10° | | 30 | Od-23 | S = MB, A' = 1,3-cyclo- hexadiene. k derived using $k_{A'} = *3.5 \times 10^6$ dm³ mol ⁻¹ s ⁻¹ [A3.8] and $k_d = *1.2 \times 10^4$ s ⁻¹ [1.4.2]. | Taim.76F921 |
| 15.20.1 | CH ₂ Cl ₂ | 4.3 × 10° | | 30 | Od-23 | S = MB, A' = TME. k derived using $k_{A'}$ = $4.0 \times 10^7 \text{ dm}^3 \text{ mol}^{-1}$ s ⁻¹ [2.35.3] and k_d = $*1.2 \times 10^4 \text{ s}^{-1}$ [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 | $\beta (k_d/k)$ /mol dm ⁻³ | t /°C | Method | Comments | Ref. |
|--------|---|--|--|---------------------------------------|----------|-----------------------|---|-------------|
| 15.20. | 2 | CH ₂ Cl ₂ | 5.4 × 10 ⁹ | | 30 | Od-23 | S = MB, A' = Rub. k derived using $k_{A'}$ = $5.3 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [3.63.3] and k_{d} = | Taim.76F921 |
| 15.21 | sodium dodecyl sulfate micelles (SDS) | H ₂ O | 1.0 × 10° | | 40 | A'd-23 | *1.2 \times 10 ⁴ s ⁻¹ [1.4.2]. 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 tri- methyl ammonium micelles (DTAC) | | 1.7×10^{8} | | 40 | A'd-23 | S = Py, A' = DPBF, Q = NaN ₃ . k derived using $k_d = 5.0 \times 10^5 \text{ s}^{-1}$ [1.1]. S and A' solubilized in DTAC micelles. | Miyo.78A174 |
| 15.23 | trimethyl phosphite (CH ₃ O) ₃ F | Me₂CO | $k_{\rm r}=1.6\times10^7$ | | rt | Pa-17 P'a (sep) | S = RB, A' = triethyl phosphite. Measured $(k_r/k_r^{A'}) = 0.65$. k_r derived using $k_r^{A'} = k_{A'} = 2.45 \times 10^7 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [15.24]. | Bold.74F495 |
| 15.23. | 1 | C ₆ H ₆ /Me (4:1) v:v | OH 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 ₃ CH ₂ | O) ₃ P (4:1) v:v | OH 2.45 × 10 ⁷ | | rt | Pa-19 | S = MB, $A' = Car$. k derived using k_d (unreported) and k_A (unreported). | Bold.74F495 |
| 15.25 | tributyl phosphite [CH ₃ (CH ₃ | Me ₂ CO | relative rates see $k_{\rm r} = 1.9 \times 10^7$ | 15.25, 15.26. | rt | Pa-17 P'a (sep) | S = RB, A' = triethyl- phosphite. Measured $(k_r/k_r^{A'}) = 0.78$. k_r derived using $k_r^{A'} = k_{A'} = 2.45 \times 10^7 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [15.24]. | Bold.74F495 |
| 15.26 | tri <i>cyclo</i> hexyl phosphite (<i>cyclo</i> -C ₆ H ₁₂ O) ₃ P | Me ₂ CO | $k_{\rm r}=1.5\times10^7$ | | rt | Pa-17 P'a (sep) | S = RB, A' = triethyl- phosphite. Measured $(k_r/k_r^{A'}) = 0.60$. k_r derived using $k_r^{A'} = k_{A'} = 2.45 \times 10^7 \text{ dm}^3$ mol ⁻¹ s ⁻¹ [15.24]. | Bold.74F495 |
| 15.27 | triphenyl phosphine (C ₆ H ₅) ₃ P | МеОН | 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 | МеОН | 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 |

References to Tables

- 34F004 Bowen, E.J., Steadman, F., The photo-oxidation of rubrene, J. Chem. Soc. 1098-101 (1934).
- 53F004 Bowen, E.J., Reactions in the liquid phase photochemistry of anthracene. Part I. The photo-oxidation of anthracenes in solution, Discuss. Faraday Soc. (14): 143-6 (1953).
- 55F004 Bowen, E.J., Tanner, D.W., The photochemistry of anthracenes. Part 3. Inter-relations between fluorescence quenching, dimerization, and photo-oxidation, Trans. Faraday Soc. 51: 475-81 (1955).
- 56F005 Livingston, R., Owens, K.E., A diffusion-controlled step in chlorophyll-sensitized photochemical autooxidations, J. Am. Chem. Soc. 78(14): 3301-5 (1956).
- 57F008 Schenck, G.O., Gollnick, K., Neumueller, O.A., Zur photosensibilisierten Autoxydation der Steroide. Darstellung von Steroid-Hydroperoxyden Mittels Phototoxischer Photosensibilisatoren, Ann. Chem. 603: 46-59 (1957).
- 58F002 Schenck, G.O., Neumueller, O.A., Zur photosensibilisierten Autoxydation der Steroide. Synthese tertiaerer Steroid-Hydroperoxyde, insbesondere des Δ^6 -Allopregnen-3 β -ol-20-on-5 α -Hydroperoxyds, Ann. Chem. **618**: 194-201 (1958).
- 58F003 Schenck, G.O., Schulte-Elte, K.-H., Photosensibilisierte Synthese tertiaerer Allylhydroperoxyde aus symmetrisch tetrasubstituierten Aethylenen, Ann. Chem. **618**: 185-93 (1958).
- 58F004 Schenck, G.O., Gollnick, K., Cinetique et inhibition de reactions photosensibilisees en presence d'oxygene moleculaire, J. Chim. Phys. Phys.-Chim. Biol. 55: 892-8 (1958).
- 59F003 Livingston, R., Rao, V.S., A further study of the photochemical autooxidation of anthracenes, J. Phys. Chem. 63: 794-9 (1959).
- 61F008 Sluyterman, L.A.E., Photo-oxidation, sensitised by proflavine, of furfuryl alcohol, N-allyl thiourea and histidine, Recl. Trav. Chim. Pays-Bas 80: 989-1002 (1961).
- 62F005 Gollnick, K., Chemismus und Kinetik der durch Xanthenfarbstoffe photosensibilisierten O₂-Uebertragungen. (Analyse der Beteiligung angeregter Singulett- und Triplettzustaende sowie der Natur der Terminationsprozesse), Ph.D., Thesis, Univ. Goettingen, 1962, 144p..
- 65F028 Kopecky, K.R., Reich, H.J., Reactivities in photosensitized olefin oxidations, Can. J. Chem. 43: 2265-70 (1965).
- 65F029 Weil, L., On the mechanism of the photo-oxidation of amino acids sensitized by methylene blue, Arch. Biochem. Biophys. 110: 57-68 (1965).
- 66F041 Wilson, T., Excited singlet molecular oxygen in photooxidation, J. Am. Chem. Soc. 88(13): 2898-902 (1966).
- 66F197 Glad, B.W., Spikes, J.D., Quantum yield studies of the dyesensitized photoinactivation of trypsin, Radiat. Res. 27: 237-49 (1966).
- 68F282 Foote, C.S., Photosensitized oxygenations and the role of singlet oxygen, Acc. Chem. Res. 1: 104-10 (1968).
- 68F284 Foote, C.S., Denny, R.W., Chemistry of singlet oxygen. VII. Quenching by β-carotene, J. Am. Chem. Soc. 90(22): 6233-5 (1968).
- 68F285 Ouannes, C., Wilson, T., Quenching of singlet oxygen by tertiary aliphatic amines. Effect of DABCO, J. Am. Chem. Soc. 90(23): 6527-8 (1968).
- 68F287 Koizumi, M., Usui, Y., Reactions by singlet oxygen and via transient complex (between dye and oxygen), produced simultaneously through the interaction between triplet eosine and oxygen, Tetrahedron Lett. (57): 6011-4 (1968).
- 68F288 Koch, E., Zur Photosensibilisierten Sauerstoffuebertragung.
 Untersuchung der Terminationsschritte durch Belichtungen bei tiefen Temperaturen, Tetrahedron 24: 6295-318 (1968).
- 68F289 Gollnick, K., Type II photosensitized oxygenation reactions, Adv. Chem. Ser. 77: 78-101 (1968).
- 68F292 Higgins, R., Foote, C.S., Cheng, H., Chemistry of singlet oxygen. V. Reactivity and kinetic characterization, Adv. Chem. Ser. 77: 102-17 (1968).
- 69F388 Stevens, B., Algar, B.E., The photoperoxidation of unsaturated organic molecules. IV. The photosensitized reaction, J. Phys. Chem. 73(6): 1711-5 (1969).

- 70E079 Algar, B.E., Stevens, B., The photoperoxidation of unsaturated organic molecules. VI. The inhibited reaction, J. Phys. Chem. 74(16): 3029-34 (1970).
- 70F188 Foote, C.S., Chang, Y.C., Denny, R.W., Chemistry of singlet oxygen. X. Carotenoid quenching parallels biological protection, J. Am. Chem. Soc. 92(17): 5216-8 (1970).
- 70F200 Richardson, W.H., Hodge, V., 1,2 Cycloaddition of singlet oxygen to 9,9'-bifluorenylidene, J. Org. Chem. 35(4): 1216-7 (1970).
- 70F250 Bethell, D., Wilkinson, R.G., Photo-oxidation of carbanions: The reactivity of singlet oxygen with 9-benzenesulphonylfluoren-9-yl anion, Chem. Commun. (18): 1178-9 (1970).
- 70F387 Matheson, I.B.C., Lee, J., Reaction of chemical acceptors with singlet oxygen produced by direct laser excitation, Chem. Phys. Lett. 7(4): 475-6 (1970).
- 70F454 Saito, I., Kato, S., Matsuura, T., Photoinduced reactions. XL. Addition of singlet oxygen to monocyclic aromatic ring, Tetra-hedron Lett. (3): 239-42 (1970).
- 70F732 Jori, G., Cauzzo, G., Proflavine-sensitized photooxidation of methionine, Photochem. Photobiol. 12: 231-7 (1970).
- 70F733 Bartlett, P.D., Mendenhall, G.D., Schaap, A.P., Competitive modes of reaction of singlet oxygen, Ann. New York Acad. Sci. 171: 79-87 (1970).
- 70F734 Foote, C.S., Denny, R.W., Weaver, L., Chang, Y., Peters, J., Quenching of singlet oxygen, Ann. New York Acad. Sci. 171: 139-45 (1970).
- 71E034 Becker, K.H., Groth, W., Schurath, U., The quenching of metastable $O_2(^1\Delta_q)$ and $O_2(^1\Sigma_g^+)$ molecules, Chem. Phys. Lett. 8: 259–62(1971).
- 71F299 Pouyet, B., Chapelon, R., Cinetique d'oxydation de l'aniline par l'oxygene singulet forme a partir d'aniline a l'etat triplet, C. R. Hebd. Seances Acad. Sci., Ser. C 272(21): 1753-6 (1971).
- 71F356 Foote, C.S., Denny, R.W., Chemistry of singlet oxygen. XIII. Solvent effects on the reaction with olefins, J. Am. Chem. Soc. 93(20): 5168-71 (1971).
- 71F398 Young, R.H., Wehrly, K., Martin, R.L., Solvent effects in dyesensitized photooxidation reactions, J. Am. Chem. Soc. 93(22): 5774-9 (1971).
- 71F403 Ishibe, N., Odani, M., Sunami, M., Photo-oxygenation of 4H-pyran-4-thiones and 4H-thiopyran-4-thiones: Reactivity and kinetic characterization, J. Chem. Soc. Pt. B (9): 1837-40 (1971).
- 71F577 Foote, C.S., Denny, R.W., Chemistry of singlet oxygen. XII. Electronic effects on rate and products of the reaction with olefins, J. Am. Chem. Soc. 93(20): 5162-7 (1971).
- 71F580 Foote, C.S., Peters, J.W., Photooxidation of sulfides, 23d. Internat. Congr. Pure Appl. Chem., Special Lectures, London, Butterworths, 1971, Vol. 4, p. 129-54..
- 71F581 Matsuura, T., Horinaka, A., Yoshida, H., Butsugan, Y., Photo-induced reactions-XLIX. Photosensitized oxygenation of cis, cis-1,5-cyclooctadiene and cis-cyclooctene, Tetrahedron 27: 3095-100 (1971).
- 71M325 Merkel, P.B., Kearns, D.R., Direct measurement of the lifetime of ¹Δ oxygen in solution, Chem. Phys. Lett. 12(1): 120-22 (1971).
- 72A019 Grams, G.W., Eskins, K., Dye-sensitized photooxidation of tocopherols. Correlation between singlet oxygen reactivity and vitamin E activity, Biochemistry 11(4): 606-8 (1972).
- 72A020 Saito, I., Imuta, M., Matsuura, T., Photoinduced reactions. LIX. Reactivity of singlet oxygen toward methoxybenzenes, Tetrahedron 28: 5307-11 (1972).
- 72F026 Merkel, P.B., Kearns, D.R., Remarkable solvent effects on the lifetime of ¹Δ_g oxygen, J. Am. Chem. Soc. 94(3): 1029-30 (1972).
- 72F027 Merkel, P.B., Nilsson, R., Kearns, D.R., Deuterium effects on singlet oxygen lifetimes in solutions. A new test of singlet oxygen reactions, J. Am. Chem. Soc. 94(3): 1030-1 (1972).
- 72F028 Foote, C., Peterson, E.R., Lee, K.-W., Chemistry of singlet oxygen. XVI. Long lifetime of singlet oxygen in carbon disulfide, J. Am. Chem. Soc. 94(3): 1032-3 (1972).
- 72F116 Yamase, T., Kokado, H., Inoue, E., The dye-sensitized photooxygenation of hexamethyleneammonium hexamethylenedithiocarbamate by xanthene dyes, Bull. Chem. Soc. Jpn. 45(3): 726-31 (1972).
- 72F126 Adams, D.R., Wilkinson, F., Lifetime of singlet oxygen in liquid

- solution, J. Chem. Soc., Faraday Trans. 2 68(4): 586-93 (1972).
- 72F196 Stevens, B., Mills, L.E., The photoperoxidation of unsaturated organic molecules. Intersystem crossing in 9,10-diphenylanthracene, Chem. Phys. Lett. 15(3): 381-2 (1972).
- 72F260 Merkel, P.B., Kearns, D.R., Radiationless decay of singlet molecular oxygen in solution. An experimental and theoretical study of electronic-to-vibrational energy transfer, J. Am. Chem. Soc. 94(21): 7244-53 (1972).
- 72F319 Carlsson, D.J., Mendenhall, G.D., Suprunchuk, T., Wiles, D.M., Singlet oxygen (¹Δ_e) quenching in the liquid phase by metal(II) chelates, J. Am. Chem. Soc. 94(25): 8960-2 (1972).
- 72F510 Young, R.H., Martin, R.L., Chinh, N., Mallon, C., Kayser, R.H., Substituent effects in dye-sensitized photooxidation reactions of furans, Can. J. Chem. 50: 932-8 (1972).
- 72F512 Smith, W.F.,Jr., Kinetic evidence for both quenching and reaction of singlet oxygen with triethylamine in pyridine solution, J. Am. Chem. Soc. 94(1) 186-90 (1972).
- 72F513 Matheson, I.B.C., Lee, J., Quenching of photophysically formed singlet $(^{1}\Delta_{p})$ oxygen in solution by amines, J. Am. Chem. Soc. **94**(10): 3310-3 (1972).
- 72F514 Young, R.H., Martin, R.L., On the mechanism of quenching of singlet oxygen by amines, J. Am. Chem. Soc. 94(15): 5183-5 (1972).
- 72F515 Hasty, N., Merkel, P.B., Radlick, P., Kearns, D.R., Role of azide in singlet oxygen reactions: reaction of azide with singlet oxygen, Tetrahedron Lett. (1): 49-52 (1972).
- 72F516 Nilsson, R., Merkel, P.B., Kearns, D.R., Unambiguous evidence for the participation of singlet oxygen (¹Δ) in photodynamic oxidation of amino acids, Photochem. Photobiol. 16: 117-24 (1972).
- 72F517 Young, R.H., Feriozi, D.T., The reactivity of isobenzofuran, J. Chem. Soc. Chem. Commun. 841-2 (1972).
- 72F518 Dalle, J.P., Magous, R., Mousseron-Canet, M., Inhibition de l'oxygene singulet, Photochem. Photobiol. 15: 411-9 (1972).
- 72F519 Martin, R.L., An investigation of reaction and quenching mechanisms of singlet molecular oxygen, Ph.D., Thesis, Georgetown Univ., Wash. D.C., 1972, 330p..
- 72F520 Matsuura, T., Yoshimura, N., Nishinaga, A., Saito, I., Photo-induced reactions. LVI. Participation of singlet oxygen in the hydrogen abstraction from a phenol in the photosensitized oxygenation, Tetrahedron 28: 4933-8 (1972).
- 72F521 Olmsted, J.,III, Karal, G., Iodine-sensitized photoformation of singlet oxygen, J. Am. Chem. Soc. 94(10): 3305-13 (1972).
- 72M077 Matheson, I.B.C., Lee, J., The lifetime of $(^1\Delta_g)$ oxygen in solution, Chem. Phys. Lett. 14(3): 350-1 (1972).
- 72R087 Schmidt, H., Rosenkranz, P., On the participation of singlet oxygen in the acridine orange sensitized photoinactivation of lysozyme, Z. Naturforsch. Teil B 27(11): 1436-7 (1972).
- 73E061 Young, R.H., Martin, R.L., Feriozi, D., Brewer, D., Kayser, R., On the mechanism of quenching of singlet oxygen by amines. III. Evidence for a charge-transfer-like complex, Photochem. Photobiol. 17(4): 233-44 (1973).
- 73F014 Young, R.H., Brewer, D., Keller, R.A., The determination of rate constants for reaction and lifetimes of singlet oxygen in solution by a flash photolysis technique, J. Am. Chem. Soc. 95(2): 375-9 (1973).
- 73F202 Kramer, H.E.A., Maute, A., Sensitized photooxygenation: Change from the Type I (radical) to Type II (singlet oxygen) mechanism, Photochem. Photobiol. 17(6): 413-23 (1973).
- 73F333 Guillory, J.P., Cook, C.F., Energy transfer processes involving ultraviolet stabilizers. Quenching of singlet oxygen, J. Polym. Sci., Polym. Chem. Ed. 11(8): 1927-37 (1973).
- 73F334 Flood, J., Russell, K.E., Wan, J.K.S., Quenching of singlet molecular oxygen by polyolefin additives in carbon disulfide solution, Macromolecules 6(5): 669-71 (1973).
- 73F438 Farmilo, A., Wilkinson, F., On the mechanism of quenching of singlet oxygen in solution, Photochem. Photobiol. 18(6): 447-50 (1973).
- 73F479 Carmier, J.-C., Deglise, X., Etude cinetique de l'oxydation photosensibilisee d'aldehydes α-ethyleniques en phase liquide a 10°C, C. R. Hebd. Seances Acad. Sci., Ser. C 277(22): 1187-9 (1973).

- 73F659 Stevens, B., Kinetics of photoperoxidation in solution, Acc. Chem. Res. 6: 90-6 (1973).
- 73F660 Olmsted, J., III, Akashah, T., Photooxidation of isobenzofurans. A dual mechanism process, J.Am. Chem. Soc. **95**(19): 6211-5 (1973).
- 73F662 Hasty, N. M., Kearns, D. R., Mechanism of singlet oxygen reactions with dienes, J. Am. Chem. Soc. 95(10): 3380-1 (1973).
- 73F664 Jefford, C.W., Boschung, A.F., Moriarty, R.M., Rimbault, C.G., Laffer, M.H., The reaction of singlet oxygen with α and β -pinenes, Helv. Chim. Acta **56**(7): 2649-59 (1973).
- 73P066 Carlsson, D.J., Suprunchuk, T., Wiles, D.M., The possible importance of singlet oxygen quenching reactions in the photostabilization of polyolefins, J. Polym. Sci., Polym. Lett. Ed. 11(1): 61-5 (1973).
- 73R045 Kepka, A.G., Grossweiner, L.I., Photodynamic inactivation of lysozyme by eosin, Photochem. Photobiol. 18(1): 49-61 (1973).
- 74F042 Mathews-Roth, M.M., Wilson, T., Fujimori, E., Krinsky, N.I., Carotenoid chromophore length and protection against photosensitization, Photochem. Photobiol. 19(3): 217-22 (1974).
- 74F044 Usui, Y., Kamogawa, K., A standard system to determine the quantum yield of singlet oxygen formation in aqueous solution, Photochem. Photobiol. 19(3): 245-7 (1974).
- 74F102 Matheson, I.B.C., Lee, J., Yamanashi, B.S., Wolbarsht, M.L., Measurement of the absolute rate constants for singlet molecular oxygen(¹Δ_g) reaction with 1,3-diphenylisobenzofuran and physical quenching by ground state molecular oxygen, J. Am. Chem. Soc. 96(11): 3343-8 (1974).
- 74F103 Matheson, I.B.C., Curry, N.U., Lee, J., Reaction rate of bilirubin with singlet oxygen (${}^{1}\Delta_{g}$) and its strong enhancement by added base, J. Am. Chem. Soc. **96**(11): 3348-51 (1974).
- 74F207 Stevens, B., Perez, S.R., The photoperoxidation of unsaturated organic molecules. X. Solvent effect on O₂¹Δ acceptor reactivity, Mol. Photochem. 6(1): 1-7 (1974).
- 74F312 Stevens, B., Perez, S.R., Ors, J.A., Photoperoxidation of unsaturated organic molecules. XIV. O₂ ¹\(\Delta_g\) acceptor properties and reactivity, J. Am. Chem. Soc. 96(22): 6846-50 (1974).
- 74F341 Carlsson, D.J., Suprunchuk, T., Wiles, D.M., The quenching of singlet oxygen $(^{1}\Delta_{g})$ by transition metal chelates, Can. J. Chem. **52**(22): 3728-37 (1974).
- 74F495 Bolduc, P.R., Goe, G.L., Singlet oxygen oxidation of phosphites to phosphates, J. Org. Chem. 39(21): 3178-9 (1974).
- 74F640 Young, R.H., Brewer, D., Kayser, R., Martin, R., Feriozi, D., Keller, R.A., On the mechanism of quenching by amines: A new method for investigation of interactions with triplet states, Can. J. Chem. 52: 2889-93 (1974).
- 74F641 Stevens, B., Perez, S.R., Small, R.D., The photoperoxidation of unsaturated organic molecules. IX. Lipoic acid inhibition of rubrene autoperoxidation, Photochem. Photobiol. 19: 315-6 (1974).
- 74F642 Carlsson, D.J., Wiles, D.M., Importance of singlet oxygen in the degradation of rubbers and plastics, Rubber Chem. Technol. 47(4): 991-1004 (1974).
- 74F643 Nilsson, R., Kearns, D.R., Role of singlet oxygen in some chemiluminescence and enzyme oxidation reactions, J. Phys. Chem. 78(17): 1681-3 (1974).
- 74F645 Hrdlovic, P., Danecek, J., Karvas, M., Durmis, J., Study of the quenching of triplet carbonyl groups and singlet oxygen by light stabilizers, Chem. Zvesti 28(6): 792-801 (1974).
- 74F646 Brewer, D.R.,III, A kinetic investigation of the generation and decay of singlet oxygen in dye sensitized systems. Part 1, Ph.D., Thesis, Georgetown Univ., Wash. D.C., 1974, 694p..
- 74F647 Jefford, C.W., Boschung, A.F., Reaction of singlet oxygen with 2-methylnorborn-2-ene, 2-methylidenenorbornane, and their 7,7-dimethyl derivatives. The transition state geometry for hydroperoxidation, Helv. Chim. Acta 57(7): 2242-57 (1974).
- 74F648 Casagrande, M., Gennari, G., Cauzzo, G., Photosensitized oxidation of di-n-butyl sulphide, Gazz. Chim. Ital. 104: 1251-7 (1974)
- 74F649 Stevens, B., Ors, J.A., Pinsky, M.L., The photo-peroxidation of unsaturated organic molecules. O₂ $^{1}\Delta_{\rm g}$ -acceptor re-encounter probabilities, Chem. Phys. Lett. **27**(2): 157-60 (1974).

- 74R112 Fahrenholtz, S.R., Doleiden, F.H., Trozzolo, A.M., Lamola, A.A., On the quenching of singlet oxygen by α-tocopherol, Photochem. Photobiol. 20(6): 505-9 (1974).
- 74R113 Foote, C.S., Ching, T.-Y., Geller, G.G., Chemistry of singlet oxygen. XVIII. Rates of reaction and quenching of α-tocopherol and singlet oxygen, Photochem. Photobiol. 20(6): 511-3 (1974).
- 74R114 Stevens, B., Small, R.D.,Jr., Perez, S.R., The photoperoxidation of unsaturated organic molecules. XIII. $O_2^{-1}\Delta_g$ quenching by α -tocopherol, Photochem. Photobiol. **20**(6): 515–7 (1974).
- 74R115 Doleiden, F.H., Fahrenholtz, S.R., Lamola, A.A., Trozzolo, A.M., Reactivity of cholesterol and some fatty acids toward singlet oxygen, Photochem. Photobiol. 20(6): 519-21 (1974).
- 74R214 Porter, D.J.T., Ingraham, L.L., Concerning the formation of singlet O₂ during the decomposition of H₂O₂ by catalase, Biochim. Biophys. Acta 334: 97-102 (1974).
- 75E223 Brauer, H.-D., Wagener, H., Untersuchung der selbstsensibilisierten Photooxidation des Rubrens in verschiedenen Loesungsmitteln, Ber. Bunsenges. Phys. Chem. 79(7): 597-604 (1975).
- 75F088 Long, C.A., Kearns, D.R., Radiationless decay of singlet molecular oxygen in solution. II. Temperature dependence and solvent effects, J. Am. Chem. Soc. 97(8): 2018-20 (1975).
- 75F147 Matheson, I.B.C., Etheridge, R.D., Kratowich, N.R., Lee, J., The quenching of singlet oxygen by amino acids and proteins, Photochem. Photobiol. 21(3): 165-71 (1975).
- 75F166 Smith, W.F.,Jr., Herkstroeter, W.G., Eddy, K.L., Quenching of singlet molecular oxygen in solution by azomethine dyes, J. Am. Chem. Soc. 97(10): 2764-70 (1975).
- 75F445 Ivanov, V.B., Shlyapintokh, V.Ya., Khvostach, O.M., Shapiro, A.B., Rozantsev, E.G., Kinetics and mechanism of nitroxyl radical formation during sensitized amine oxidation, J. Photochem. 4(5/6): 313-9 (1975).
- 75F485 Poppe, W., Grossweiner, L.I., Photodynamic sensitization by 8-methoxypsoralen via the singlet oxygen mechanism, Photochem. Photobiol. 22(5): 217-9 (1975).
- 75F558 Stevens, B., Williams, R.R., An experimental approach to the estimation of diffusive displacement parameters for bimolecular reactions in solution, Chem. Phys. Lett. 36(1): 100-5 (1975).
- 75F578 Rosenthal, I., Singlet molecular oxygen and superoxide radical anion, Isr. J. Chem. 13(2): 86-90 (1975).
- 75F623 Nathu Ram, Bansal, W.R., Uppal, S.S., Sidhu, K.S., Reactions of singlet oxygen III. Dye sensitized oxidation of phenothiazine, Proceedings of the Symposium on Singlet Molecular Oxygen, Bhabha At. Res. Cent., Bombay, 10-13 Feb 1975, p.141-52.
- 75F652 Lightner, D.A., Pak, C.-S., Dye-sensitized photooxygenation of tert-butylpyrroles, J. Org. Chem. 40(19): 2724-8 (1975).
- 75F653 Ching, T.-Y., Foote, C.S., Chemistry of singlet oxygen. XXII. Photooxidation of nitrones, Tetrahedron Lett. (44): 3771-4 (1975).
- 75F654 Bystritskaya, E.V., Karpukhin, O.N., Effect of the aggregate state of the medium on singlet oxygen quenching, Dokl. Phys. Chem. 221(4-6): 353-6 (1975).
- 75F655 Zolotoi, N.B., Karpov, G.V., Skurat, V.E., New method for the mass spectrometric study of the kinetics of molecular oxygen consumption in liquid-phase photooxidation processes, Kinet. Catal. 16(6): 1229-34 (1975).
- 75F656 Foote, C.S., Dzakpasu, A.A., Lin, J.W.-P., Chemistry of singlet oxygen. XX. Mechanism of the sensitized photooxidation of enamines, Tetrahedron Lett. (14): 1247-50 (1975).
- 75P063 Zweig, A., Henderson, W.A.,Jr., Singlet oxygen and polymer photooxidations. I. Sensitizers, quenchers, and reactants, J. Polym. Sci., Polym. Chem. Ed. 13(3): 717-36 (1975).
- 75R071 Foote, C.S., Ching, T.-Y., Chemistry of singlet oxygen. XXI. Kinetics of bilirubin photooxygenation, J. Am. Chem. Soc. 97(21): 6209-14 (1975).
- 76E072 Guiraud, H.J., Foote, C.S., Chemistry of superoxide ion. III. Quenching of singlet oxygen, J. Am. Chem. Soc. 98(7): 1984-6 (1976).
- 76F041 Brkic, D., Forzatti, P., Pasquon, I., Trifiro, F., Kinetic aspects of dye-sensitized photo-oxygenation, J. Photochem. 5(1): 23-32 (1976).

- 76F071 Byers, G.W., Gross, S., Henrichs, P.M., Direct and sensitized photooxidation of cyanine dyes, Photochem. Photobiol. 23(1): 37– 43 (1976).
- 76F105 Schmidt, H., Rosenkranz, P., On the mechanism of the acridine orange sensitized photodynamic inactivation of lysozyme. I. Basic kinetics, Z. Naturforsch., C, Biosci. 31(1-2): 29-39 (1976).
- 76F126 Rosenthal, I., Frimer, A., The quenching effect of iodide ion on singlet oxygen, Photochem. Photobiol. 23(3): 209-11 (1976).
- 76F197 Wamser, C.C., Herring, J.W., Photooxidation of benzophenone oxime and derivatives, J. Org. Chem. 41(8): 1476-7 (1976).
- 76F232 Foote, C.S., Thomas, M., Ching, T.-Y., Photooxidation of phenols, J. Photochem. 5(2): 172 (1976).
- 76F247 Gorman, A.A., Lovering, G., Rodgers, M.A.J., The photosensitized formation and reaction of singlet oxygen, O₂*(¹Δ), in aqueous micellar systems, Photochem. Photobiol. 23(6): 399-403 (1976).
- 76F417 Evans, D.F., Tucker, J.N., Reactivity of the $(^{1}\Delta_{g})_{2}$ and $^{1}\Delta_{g}$ states of oxygen produced by direct laser excitation, J. Chem. Soc., Faraday Trans. 2 **72**(9): 1661-6 (1976).
- 76F422 Stevens, B., Ors, J.A., Photoperoxidation of unsaturated organic molecules. 16. Excitation energy fission, J. Phys. Chem. 80(20): 2164-5 (1976).
- 76F425 Brabham, D.E., Lee, J., Excited state interactions of α-tocopherol and molecular oxygen, J. Phys. Chem. 80(20): 2292-6 (1976).
- 76F570 Wagener, H., Brauer, H.-D., Photoperoxidation of heterocoerdianthrone in different solvents, Mol. Photochem. 7(4): 441-64 (1976).
- 76F662 Matheson, I.B.C., Lee, J., The non-chemiluminescent reaction of luminol with singlet oxygen, Photochem. Photobiol. 24(6): 605-7 (1976).
- 76F900 Singh, P., Ullman, E.F., Nitroso compounds and azo dioxides as quenchers of singlet oxygen ($^{1}\Delta_{g}$) and sensitizer triplet states, J. Am. Chem.Soc. **98**(10): 3018–9 (1976).
- 76F902 Wilkinson, F., Physical properties of singlet oxygen in fluid solvents, Singlet Oxygen, Reactions with Organic Compounds and Polymers, B. Ranby and J.F. Rabek (eds.), John Wiley & Sons, New York, N.Y., 1976, p.27-35.
- 76F903 Young, R.H., Brewer, D.R., The mechanism of quenching of singlet oxygen, Singlet Oxygen, Reactions with Organic Compounds and Polymers, B. Ranby and J.F. Rabek (eds.), John Wiley & Sons, New York, N.Y., 1976, p.36-47.
- 76F909 Chaineaux, J., Tanielian, C., Singlet oxygen reactions with polyisoprene model molecules: 4-methyl-4-octene and 4,8-dimethyl-4,8-dodecadiene, Singlet Oxygen, Reactions with Organic Compounds and Polymers, B. Ranby and J.F. Rabek (eds.), John Wiley & Sons, New York, N.Y., 1976, p.164-73.
- 76F910 Rosenkranz, P., Al-Ibrahim, A., Schmidt, H., Mechanism of the dye-sensitized photodynamic inactivation of lysozyme, Singlet Oxygen, Reactions with Organic Compounds and Polymers, B. Ranby and J.F. Rabek (eds.), John Wiley & Sons, New York, N.Y., 1976, p.195-202.
- 76F921 Taimr, L., Pospisil, J., Antioxidants and stabilizers. LXV. Contribution to the investigation of sensitized photooxidation of phenolic antioxidants. Quenching of singlet oxygen with stilbenequinoid compounds, Angew. Makromol. Chem. 52: 31-8 (1976).
- 76R011 Stevens, B., Small, R.D.,Jr., The photoperoxidation of unsaturated organic molecules. XV. O₂ ¹\Delta_g quenching by bilirubin and biliverdin, Photochem. Photobiol. 23(1): 33-6 (1976).
- 77F055 Davidson, R.S., Trethewey, K.R., Concerning the use of amines as probes for participation of singlet oxygen in dye-sensitised oxygenation reactions, J. Chem. Soc., Perkin Trans. 2 (2): 178-82 (1977).
- 77F074 Rohatgi-Mukherjee, K.K., Gupta, A.K., Anthracene sulphonate sensitized photooxidation of iodide ion in aqueous solution via singlet oxygen, Chem. Phys. Lett. **46**(2): 368-71 (1977).
- 77F113 Bethell, D., McKeivor, R., Intermediates in the decomposition of aliphatic diazo-compounds. Part 13. Mechanistic studies on the reaction of diaryldiazomethanes with singlet molecular oxygen, J. Chem. Soc., Perkin Trans. 2 (3): 327-33 (1977).

- 77F129 Matheson, I.B.C., Toledo, M.M., The singlet oxygen reactivity of biliverdin, Photochem. Photobiol. 25(3): 243-8 (1977).
- 77F162 Bortolus, P., Dellonte, S., Beggiato, G., Corio, W., Interaction between singlet oxygen (¹Δ_g) and model compounds for polymers. A flash photolytic study, Eur. Polym. J. 13(3): 185-8 (1977).
- 77F176 Drews, W., Schmidt, R., Brauer, H.-D., Die Kinetik der selbstsensibilisierten Photooxidation des Heterocoerdianthrons im bereich niedriger Konzentrationen, J. Photochem. 6(6): 391-403 (1976/77).
- 77F240 Rosenthal, I., Bercovici, T., Frimer, A., Dye sensitized photo-oxidation of chlorpromazine, J. Heterocycl. Chem. 14(2): 355-7 (1977).
- 77F378 Terao, J., Matsushita, S., Products formed by photosensitized oxidation of unsaturated fatty acid esters, J. Am. Oil Chem. Soc. 54(6): 234-8 (1977).
- 77F433 Sysak, P.K., Foote, C.S., Ching, T.-Y., Chemistry of singlet oxygen. XXV. Photooxygenation of methionine, Photochem. Photobiol. 26(1): 19-27 (1977).
- 77F486 Monroe, B.M., Quenching of singlet oxygen by aliphatic amines, J. Phys. Chem. 81(19): 1861-4 (1977).
- 77F489 Seely, G.R., Mechanisms of the photosensitized oxidation of tyramine, Photochem. Photobiol. 26(2): 115-23 (1977).
- 77F645 Frimer, A.A., Bartlett, P.D., Boschung, A.F., Jewett, J.G., Reaction of singlet oxygen with 4-methyl-2,3-dihydro-γ-pyrans, J. Am. Chem. Soc. 99(24): 7977-86 (1977).
- 77F794 Fanghaenel, E., Lutze, G., Studies on the sensitized photo-oxidation of 1,3-dithiol-thiones-(2), J. Prakt. Chem. 319(6): 875-82 (1977).
- 77F858 Yamauchi, R., Matsushita, S., Quenching effect of tocopherols on the methyl linoleate photooxidation and their oxidation products, Agric. Biol. Chem. 41(8): 1425-30 (1977).
- 77F876 Faler, G.R., I. A study of the kinetics of the 1,2-cycloaddition of singlet oxygen to vinyl ethers. II. An investigation of the reaction of singlet oxygen with adamantylideneadamantane, Ph.D., Thesis, Wayne State Univ., Detroit, MI, 1977, 157p..
- 78A005 Monroe, B.M., Rates of reaction of singlet oxygen with olefins, J. Phys. Chem. 82(1): 15-8 (1978).
- 78A171 Thomas, M.J., Foote, C.S., Chemistry of singlet oxygen. XXVI. Photooxygenation of phenols, Photochem. Photobiol. 27(6): 683-93 (1978).
- 78A174 Miyoshi, N., Tomita, G., Production and reaction of singlet oxygen in aqueous micellar solutions using pyrene as photosensitizer, Z. Naturforsch., Teil B 33B(6): 622-7 (1978).
- 78A227 Held, A.M., Halko, D.J., Hurst, J.K., Mechanisms of chlorine oxidation of hydrogen peroxide, J. Am. Chem. Soc. 100(18): 5732-40 (1978).
- 78A266 Snyakin, A.P., Samsonova, L.V., Shlyapintokh, V.Ya., Ershov, V.V., Kinetics and mechanism of the interaction of sterically hindered phenols with singlet oxygen, Bull. Acad. Sci. USSR, Div. Chem. Sci. 27(1): 46-52 (1978).
- 78A275 Gupta, A.K., Singh, B.P., Rohatgi-Mukherjee, K.K., Photoperoxidation of anthracene sulphonates, J. Indian Chem. Soc. 55(4): 382-5 (1978).
- 78A278 Barboy, N., Kraljic, I., On the reactivity of singlet oxygen in aqueous micellar systems, J. Photochem. 9(4): 336-7 (1978).
- 78A338 Smith, G.J., Photo-oxidation of tryptophan sensitized by methylene blue, J. Chem. Soc., Faraday Trans. 2 74(7): 1350-4 (1978).
- 78A344 Tanielian, C., Chaineaux, J., Singlet oxygen reactions with model compounds of cis and trans polyisoprene containing two units, J. Photochem. 9(1): 19-32 (1978).
- 78A357 Tanielian, C., Chaineaux, J., Singlet oxygen reactions with 2,7-dimethyl-2,6-octadiene, Photochem. Photobiol. 28(4-5): 487-92 (1978).
- 78A360 Kraljic, I., Sharpatyi, V.A., Determination of singlet oxygen rate constants in aqueous solutions, Photochem. Photobiol. 28(4-5): 583-6 (1978).
- 78E036 Merkel, P.B., Herkstroeter, W.G., The fate of oxygen in the quenching of excited singlet states, Chem. Phys. Lett. 53(2): 350-4 (1978).

- 78E143 Matheson, I.B.C., Lee, J., King, A.D., The lifetime of singlet oxygen ($^{1}\Delta_{g}$) in heavy water, a revised value, Chem. Phys. Lett. **55**(1): 49-51 (1978).
- 78E144 Gorman, A.A., Rodgers, M.A.J., Lifetime and reactivity of singlet oxygen in an aqueous micellar system: A pulsed nitrogen laser study, Chem. Phys. Lett. 55(1): 52-4 (1978).
- 78E238 Furue, H., Russell, K.E., Deactivation of singlet oxygen and triplet pentacene by transition metal complexes, Can. J. Chem. 56(12): 1595-601 (1978).
- 78E263 Gorman, A.A., Lovering, G., Rodgers, M.A.J., A pulse radiolysis study of the triplet sensitized production of singlet oxygen: determination of energy transfer efficiencies, J. Am. Chem. Soc. 100(14): 4527-32 (1978).
- 78F020 Kraljic, I., Kramer. H.E.A., On the reaction of singlet molecular oxygen with N-allylthiourea in aqueous solution, Photochem. Photobiol. 27(1): 9-12 (1978).
- 78F061 Usui, Y., Tsukada, M., Nakamura, H., Kinetic studies of photosensitized oxygenation by singlet oxygen in aqueous micellar solutions, Bull. Chem. Soc. Jpn. 51(2): 379-84 (1978).
- 78F149 Jefford, C.W., Rimbault, C.G., Reaction of singlet oxygen with 2-methylidenenorbornene. Evaluation of electronic and steric effects on the course of hydroperoxidation, J. Org. Chem. 43(10): 1908-12 (1978).
- 78F183 Gupta, A.K., Rohatgi-Mukherjee, K.K., Solvent effect on photosensitized oxidation of iodide ion by anthracene sulphonates, Photochem. Photobiol. 27(5): 539-43 (1978).
- 78F201 Delmelle, M., An investigation of retinal as a source of singlet oxygen, Photochem. Photobiol. 27(6): 731-4 (1978).
- 78F276 Wilkinson, F., Ho, W.-T., Electronic energy transfer from singlet molecular oxygen to carotenoids, Spectrosc. Lett. 11(7): 455-63 (1978).
- 78F286 Jefford, C.W., Rimbault, C.G., Reaction of singlet oxygen with norbornenyl ethers. Characterization of dioxetanes and evidence for zwitterionic peroxide precursors, J. Am. Chem. Soc. 100(20): 6437-45 (1978).
- 78F290 Jefford, C.W., Rimbault, C.G., Reaction of singlet oxygen with a norbornadienol ether. Intramolecular interception of a zwitterionic peroxide, J. Am. Chem. Soc. 100(20): 6515-6 (1978).
- 78F404 Koka, P., Song, P.-S., Protection of chlorophyll a by carotenoid from photodynamic decomposition, Photochem. Photobiol. 28(4-5): 509-15 (1978).
- 78F430 Rousseau, G., Le Perchec, P., Conia, J.M., Petits cycles. XL. Sur le mechanisme de formation des hydroperoxydes allyliques dans la reaction de l'oxygene singulet avec les vinylcyclopropanes, Tetrahedron 34(23): 3483-94 (1978).
- 78F438 Timpe, G.I., Klokova, E.M., El'tsov, A.V., Photosensitized oxidation of pseudoazulenes, J. Org. Chem. USSR 14(4): 625-30 (1978).
- 78F464 Schulte-Elte, K.H., Muller, B.L., Rautenstrauch, V., Preference for syn ene additions of ¹O₂ to trisubstituted, acyclic olefins, Helv. Chim. Acta 61(8): 2777-83 (1978).
- 78F474 Herlem, D., Ouannes, C., Oxydation photochimique d'une amine tertiaire: la dregamine, Bull. Soc. Chim. Fr. (11-12): I-451-4 (1978).
- 78F497 Edilashvili, I.L., Ioseliani, K.B., Dzhanibekov, N.F., Markova, E.I., Akhmed-zade, D.A., The quenching of singlet oxygen by complex salts of O,O-diarylphosphorodithioic acids, Russ. J. Phys. Chem. 52(8): 1197-8 (1978).
- 78F586 Kretschmer, G., Paquette, L.A., Concerning the inhibition of singlet oxygen attack on compounds containing urazole rings, Heterocycles 11(Special Issue): 359-62 (1978).
- 78F605 Slawinska, D., Chemiluminescence and the formation of singlet oxygen in the oxidation of certain polyphenols and quinones, Photochem. Photobiol. 28(4-5): 453-8 (1978).
- 78N003 Greenstock, C.L., Wiebe, R.H., Photosensitized carcinogen degradation and the possible role of singlet oxygen in carcinogen activation, Photochem. Photobiol. 28(4-5): 863-7 (1978).
- 79A010 Krasnovsky, A.A.,Jr., Photoluminescence of singlet oxygen in pigment solutions, Photochem. Photobiol. 29(1): 29-36 (1979).
- 79A050 Monroe, B.M., Mrowca, J.J., Quenching of singlet oxygen by nickel complexes, J. Phys. Chem. 83(5): 591-5 (1979).

C₃H₀N

C₃H₀PO₃

 C_4H_4O

 C_4H_4S

C₄H₆O

 $C_4H_6O_2$

C4H8N2O

 $C_4H_8N_2S$

C₄H₈O

C₄H₈OS

 $C_4H_8O_2$

 C_aH_BS

 $C_4H_8S_2$

C4H9N

C4H9NO

 $C_4H_{10}N_2$

 $C_4H_{10}O$

 $C_4H_{10}O_2S$

 $C_4H_{10}S$

 $C_4H_{10}S_2$

 $C_4H_{11}N$

 C_4H_8

Isopropylamine 6.3

Trimethylamine 6.22

Thiophene 11.35

2-Butenal (trans) 2.32

2-Butene (cis) 2.29

2-Butene (trans) 2.30

Propene, 2-methyl- 2.21

Thiourea, N-allyl- 11.31 Ethene, ethoxy- 2.1

Furan, tetrahydro- 1.26 15.11

Acetic acid, ethyl ester 1.28 Dioxane **1.27 15.19**

Pyrrole, tetrahydro- 6.15

Thiophene, tetrahydro- 11.25

Propane, 2-methyl-2-nitroso- 13.7

2-Propanol, 2-methyl- 1.25 15.7

Sulfide, 2,2'-dihydroxydiethyl 11.16

1-Oxa-4-thiacyclohexane 11.27

Urea, N-allyl- 6.37

1,4-Dithiane 11.40

1-Butanol **1.24 15.6**

Piperazine 6.39

Ethyl ether 79E699

1-Butanethiol 11.1

Sulfide, diethyl 11.14

Butylamine 6.4

t-Butylamine 6.6

Disulfide, diethyl 11.39

2-Butene 2.31

Phosphite, trimethyl- 15.23

3,6-Dioxacyclohexene 2.55

Propylamine 6.2

Furan 5.1

| 79A085 | Monroe, | B.M., | Rates of | f reaction | of single | t oxygen | with | sulfides, |
|--------|----------|---------|------------------|------------|-----------|----------|------|-----------|
| . Pl | hotochem | . Photo | biol. 2 9 | (4): 761~ | 4 (1979) | | | |

79A086 Kacher, M.L., Foote, C.S., Chemistry of singlet oxygen. XXVIII. Steric and electronic effects on the reactivity of sulfides with singlet oxygen, Photochem. Photobiol. 29(4): 765-9 (1979).

79F074 Tanielian, C., Chaineaux, J., Singlet oxygen reactions with model compounds of cis and trans-polyisoprene containing one unit. Kinetic aspects. J. Polym. Sci., Polym. Chem. Ed. 17(3): 715-29 (1979).

79F104 Lightner, D.A., Park, Y-T., On the syntheses and singlet oxygen reactivity of oxodipyrromethene models for bilirubin. Tetrahedron 35(4): 463-71 (1979).

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.

| | | | Diethylamine 6.12 |
|---|--|------------------|---|
| Br ⁻ | Bromide ion 12.2 12.3 12.4 | | Isobutylamine 6.5 |
| CClF ₃ | Methane, chlorotrifluoro- 1.7 | C_5H_4OS | 4H-Pyran-4-thione 11.32 |
| CCl ₃ D | Chloroform-d 1.6 | $C_5H_4O_2$ | Furfural 5.4 |
| CCl ₄ | Carbon tetrachloride 1.41 1.42 1.43 1.44 1.45 1.46 | $C_5H_4O_3$ | 2-Furoic acid 5.8 |
| | 1.8 79E699 | $C_5H_4S_2$ | 4H-Thiopyran-4-thione 11.43 |
| CD_4O | Methanol-d ₄ 1a.8 | C_5H_5N | Pyridine 1.29 1a.11 5.45 79E699 |
| CHCl ₃ | Chloroform 1.5 79E699 | $C_5H_5N_5$ | Adenine 14.37 |
| CH_2Cl_2 | Methane, dichloro- 1.4 1a.10 1a.11 1a.9 | C_5H_6 | Cyclopentadiene 2.86 79A106 |
| CH_4N_2S | Thiourea 11.29 | $C_5H_6N_2O_2$ | Thymine 14.39 |
| CH ₄ O | Methanol 1.3 1.38 1.39 1.40 1.41 1.42 1.43 1.44 | C_5H_6O | Furan, 2-methyl- 5.2 |
| | 1.45 1.46 1.47 1.49 1.50 15.2 la.10 la.11 la.9 | $C_5H_6O_2$ | Furan, 2-methoxy- 5.5 |
| CS_2 | Carbon disulfide 1.47 1.9 | | Furfuryl alcohol 5.6 |
| $C_2Cl_3F_3$ | Ethane, 1,2,2-trichloro-1,1,2-trifluoro- 1a.2 | C_5H_7N | Furfurylamine 5.3 |
| $C_2H_2Cl_4$ | Ethane, 1,1,2,2-tetrachloro- 1.18 | C_5H_8 | Cyclopentene 2.50 |
| C ₂ H ₃ Cl ₃ O | Ethanol, 2,2,2-trichloro- 1.15 | C_5H_8O | 4H-Pyran, 2,3-dihydro- 15.12 |
| $C_2H_3F_3O$ | Ethanol, 2,2,2-trifluoro- 1.16 | $C_5H_9N_3$ | Histamine 5.50 |
| C_2H_3N | Acetonitrile 1.17 | C_5H_{10} | 2-Butene, 2-methyl- 2.33 |
| $C_2H_4Cl_2$ | Ethane, 1,1-dichloro- 1.13 | | 2-Pentene (cis) 2.38 |
| C ₂ H ₄ Cl ₂ O | Ethanol, 2,2-dichloro- 1.14 | | 2-Pentene (trans) 2.39 |
| C_2H_5FO | Ethanol, 2-fluoro- 1.12 | | 1-Pentene 2.37 |
| C_2H_5I | Ethane, iodo- 15.4 | $C_5H_{10}O$ | 2-Buten-1-ol, 3-methyl- 79F137 |
| C ₂ H ₆ N ₂ S | Thiourea, N-methyl- 11.30 | $C_5H_{10}S$ | Thiacyclohexane 11.26 |
| C_2H_6O | Ethanol 1.10 1.48 15.3 79E699 | $C_5H_{11}N$ | Piperidine 6.16 |
| C ₂ H ₆ OS | Sulfoxide, dimethyl- 1a.1 | $C_5H_{11}NO_2S$ | Methionine 8.2 79A112 |
| $C_2H_6O_2$ | Ethane, 1,2-dihydroxy- 1.11 1.40 | $C_5H_{12}S$ | Sulfide, butyl methyl 11.3 |
| C_2H_7N | Ethylamine 6.1 | $C_5H_{13}NO_2$ | Methylamine, N,N-di(2-hydroxyethyl)- 6.19 |
| C_3D_6O | Acetone-d ₆ 1a.3 | C_6D_6 | Benzene- d_6 1.33 |
| $C_3H_4N_2$ | Imidazole 5.49 | C_6F_6 | Benzene, hexafluoro- 1.35 |
| C_3H_4O | 2-Propenal 2.22 | $C_6H_4O_2$ | Benzoquinone 14.1 79A106 |
| $C_3H_4O_2$ | 3,5-Dioxacyclopentene 2.51 | C_6H_5Br | Benzene, bromo- 1.34 1.50 3.2 |
| C_3H_5BrO | Propane, 1-bromo-2,3-epoxy- 1.23 | C_6H_5Cl | Benzene, chloro- 1a.5 |
| $C_3H_6NS_2^-$ | Dithiocarbamate ion, dimethyl- 11.41 | C_6H_6 | Benzene 1.32 1.49 3.1 79E699 |
| C_3H_6O | Acetone 1.22 | $C_6H_6D_6$ | 2-Butene, 2,3-dimethyl- d_6 - 79F155 |
| C_3H_6O C_3H_7Br | Propane, 1-bromo- 1.20 | C_0H_0O | Furan, 2-vinyl- 5.9 |
| | | $C_0H_0O_2$ | Furan, 2-acetyl- 5.17 |
| C_3H_7NO | Acetone oxime 13.1 | - | Hydroquinone 4.31 |
| | Formamide, <i>N</i> , <i>N</i> -dimethyl- 1.21 6.20 | C_6H_7N | Aniline 7.1 |
| $C_3H_7NO_2$ | Alanine 8.1 | C_6H_8 | 1,3-Cyclohexadiene 2.91 |
| C_3H_8O | 2-Propanol 1.19 15.5 | ~-0n | • |

| | | | • |
|-----------------------------------|---|-----------------------------------|---|
| $C_6H_8Cl_2N_2O_2$ | Cyclohexane, 1,4-dichloro-1,4-dinitroso- (cis) 13.9 | C_7H_{12} | 2-Butene, 2-cyclopropyl- (trans) 2.34 |
| | Cyclohexane, 1,4-dichloro-1,4-dinitroso- (trans) 13.8 | | Cyclohexane, methylidene- 2.7 |
| | 2,3-Diazabicyclo[2.2.2]oct-2-ene-2,3-dioxide, 1,4- | | Cyclohexene, 1-methyl- 2.56 |
| | dichloro- 13.10 | | Cyclohexene, 4-methyl- 2.57 |
| $C_6H_8N_2$ | o-Phenylenediamine 7.14 | | Cyclopentane, ethylidene- 2.6 |
| C_6H_8O | Furan, 2,4-dimethyl- 5.28 | | |
| 061180 | • | OH NO | Propene, 1-cyclopropyl-2-methyl- 2.23 |
| C II O | Furan, 2,5-dimethyl- 5.29 79A106 | $C_7H_{12}NS_2$ | Dithiocarbamate ion, hexamethylene- 11.42 |
| $C_6H_8O_2$ | Cyclohexene, 3,6-endoperoxy- 2.62 | $C_7H_{12}N_2$ | 4H-Pyrazole, tetramethyl- 79F278 |
| | Ether, furfuryl methyl 5.7 | $C_7H_{12}O$ | Ethanol, 2-cyclopentylidene- 79F137 |
| | Furfuryl alcohol, α-methyl- 5.10 | $C_7H_{13}N$ | Quinuclidine 6.38 |
| C_6H_9N | Pyrrole, 2,5-dimethyl- 5.44 | $C_7H_{13}NO$ | Δ^1 -Pyrroline-N-oxide, 2,4,4-trimethyl- 13.6 |
| C ₆ H ₉ NO | 2-Furanmethanamine, N-methyl- 5.18 | 1 13 | Δ^1 -Pyrroline-N-oxide, 4,5,5-trimethyl- 13.5 |
| , | Furfurylamine, N-methyl- 5.18 | C_7H_{14} | 1-Heptene 2.76 |
| $C_6H_9N_3O_2$ | Histidine 8.7 79A112 | C ₇ 11 ₁₄ | • |
| | | CHA | 2-Pentene, 2,4-dimethyl- 2.47 |
| C ₆ H ₉ OD | 4H-Pyran-4-d, 2,3-dihydro-4-methyl- 15.15 | $C_7H_{14}N_2$ | Diethylamine, N-(2-cyanoethyl)- 6.26 |
| C ₆ H ₉ OT | 4H-Pyran-2-t, 2,3-dihydro-4-methyl- 15.13 | $C_7H_{14}O$ | 2-Penten-1-ol, 3,4-dimethyl- 79F137 |
| | 4H-Pyran-3-t, 2,3-dihydro-4-methyl- 15.14 | | 2-Penten-1-ol, 3-ethyl- 79F137 |
| | 4H-Pyran-4-t, 2,3-dihydro-4-methyl- 15.16 | $C_7H_{15}N$ | Piperidine, 2,6-dimethyl- 6.17 |
| C_6H_{10} | Cyclohexene 2.54 | C_7H_{16} | Heptane 15.8 |
| | Cyclopentane, methylidene- 2.5 | $C_7H_{16}S$ | Sulfide, 2-butyl 1-propyl 11.18 |
| • | Cyclopentene, 1-methyl- 2.52 | 7 10 | Sulfide, 2-methyl-2-propyl 1-propyl 11.19 |
| | Cyclopropane, (dimethylmethylidene)- 79F119 | $C_7H_{17}NO$ | Diethylamine, 2-methoxyethyl- 6.25 |
| | | | |
| | 2,4-Hexadiene (trans, trans) 2.89 | $C_8F_{12}NiS_4^{2-}$ | Nickelate(II) ion, bis(hexafluoro-2,3-butanedithionato)- |
| | 1,5-Hexadiene 2.88 | | (2-)- S,S')- 10.49 |
| $C_6H_{11}D$ | 2-Pentene, 2-methyl-4d- 79F155 | C_8H_6N | Indole 79A106 |
| C_6H_{12} | 1-Butene, 2,3-dimethyl- 2.28 | C_8H_6O | Isobenzofuran 5.35 |
| | 2-Butene, 2,3-dimethyl- 2.35 | $C_8H_7N_3O_2$ | Luminol 7.20 |
| | Cyclohexane 1.30 | C_8H_8 | Styrene 3.6 |
| | 2-Hexene 2.53 | $C_8H_8Br_2$ | Cyclooctatetraene dibromide 2.117 |
| | 2-Pentene, 3-methyl- (cis) 2.42 | $C_8H_8O_2$ | Benzoic acid, methyl ester 1.37 3.5 |
| | • | | • |
| | 2-Pentene, 3-methyl- (trans) 2.43 | C_8H_{10} | Benzene, ethyl- 3.3 |
| | 2-Pentene, 4-methyl- (cis) 2.45 | | Fulvene, 6,6-dimethyl- 2.115 |
| | 2-Pentene, 4-methyl- (trans) 2.46 | | Norborna-2,5-diene, 2-methyl- 2.94a |
| | 2-Pentene, 2-methyl- 2.40 | | Norborn-5-ene, 2-methylidene- 2.94b |
| | 2-Pentene, 3-methyl- 2.44 | $C_8H_{10}BrN$ | Aniline, p-bromo-N,N-dimethyl- 7.8 |
| $C_6H_{12}N_2$ | 1,4-Diazabicyclo[2.2.2]octane 6.40 79F463 | $C_8H_{10}CIN$ | Aniline, m-chloro-N,N-dimethyl- 7.7 |
| $C_6H_{12}N_2NiS_4$ | Nickel(II), bis(N,N-dimethyldithiocarbamato-S,S')- 10.8 | $C^8H^{10}O$ | Cyclohexa-3,5-dien-1-one, 2,2-dimethyl- 2.94 |
| $C_6H_{12}N_4$ | Hexamethylenetetramine 6.41 | $C_8H_{10}OS$ | Sulfide, 4-methoxyphenyl methyl 11.12 |
| $C_6H_{12}O$ | Cyclohexanol 1.31 | $C_8H_{10}O_2$ | Benzene, 1,2-dimethoxy- 3.25 |
| C ₆ 11 ₁₂ U | • | C81110O2 | · |
| | 2-Pentene-4-ol, 2-methyl- 2.41 | | Benzene, 1,3-dimethoxy- 3.26 |
| | 2-Penten-1-ol, 3-methyl- 79F137 | | Benzene, 1,4-dimethoxy- 3.27 |
| $C_6H_{12}O_2$ | Ethene, 1,2-diethoxy- (cis) 2.3 | | Fulvene endoperoxide, 6,6-dimethyl- 2.87 |
| | Ethene, 1,2-diethoxy- (trans) 2.4 | $C_8H_{10}S$ | Sulfide, benzyl methyl 11.5 |
| | Ethene, 1,1-diethoxy- 2.2 | | Sulfide, methyl 3-methylphenyl 11.10 |
| $C_6H_{12}S$ | Thiacycloheptane 11.28 | | Sulfide, methyl 4-methylphenyl 11.11 |
| $C_6H_{13}N$ | Cyclohexylamine 6.7 | $C_8H_{11}D$ | Norbornane-3-d, endo-2-methylidene- 2.73 |
| -0 -13- | Isobutenylamine, N,N-dimethyl- 6.21 | 0 77 | Norbornane-3-d, exo-2-methylidene- 2.72 |
| | Piperidine, 1-methyl- 6.32 | $C_8H_{11}N$ | Aniline, N,N-dimethyl- 7.6 |
| CHNO | | Ogriffia | • |
| $C_6H_{14}N_4O_2$ | Arginine 8.4 | CH NO | Ethylamine, 2-phenyl- 6.9 |
| $C_6H_{14}O_2$ | Ethanol, 2-butoxy- 1a.4 | C ₈ H ₁₁ NO | Tyramine 8.6 |
| $C_6H_{14}S$ | Sulfide, diisopropyl 11.17 | $C_8H_{11}N_3O_2$ | 4H-[1,2,4]Triazolo[1,2,a]norbornane, 4-methyl-3,5- |
| | Sulfide, ethyl 2-methyl-2-propyl 11.15 | | dioxo- 5.50a |
| $C_6H_{15}N$ | Diisopropylamine 6.14 | C_8H_{12} | Cyclobutane, (cyclopropylmethylidene)- 2.11 |
| | Dipropylamine 6.13 | | Norbornane, 2-methylidene- 2.71 |
| | Triethylamine 6.23 | | Norborn-2-ene, 2-methyl- 2.64 |
| $C_6H_{15}NO$ | Diethylamine, N-(2-hydroxyethyl)- 6.24 | $C_8H_{12}NiS_4^{2-}$ | Nickelate(II) ion, bis(2,3-butanedithionato(2-)-S,S')- |
| $C_6H_{15}PO_3$ | Phosphite, triethyl- 15.24 | C8111211154 | |
| C_7H_7BrS | Sulfide, 4-bromophenyl methyl 11.9 | | 10.48 |
| | | $C_8H_{13}N$ | Pyrrole, 1-(2-methyl-2-propyl)- 5.41 |
| C_7H_7CIS | Sulfide, 3-chlorophenyl methyl 11.7 | | Pyrrole, 2-(2-methyl-2-propyl)- 5.42 |
| | Sulfide, 4-chlorophenyl methyl 11.8 | | Pyrrole, 3-(2-methyl-2-propyl)- 5.43 |
| C_7H_7FS | Sulfide, 4-fluorophenyl methyl 11.6 | Сн | 2-Butene, 2-cyclopropyl-3-methyl- 2.36 |
| C_7H_8 | Toluene 1.36 79E699 | C_8H_{14} | |
| C_7H_8O | Benzene, methoxy- 3.4 | | Cycloheptene, 1-methyl- 2.77 |
| C7H8OS | 4H-Pyran-4-thione, 2,6-dimethyl- 11.33 | | Cyclohexane, ethylidene- 2.8 |
| $C_7H_8O_6$ | Ascorbic acid 14.2 | | Cyclohexene, 1,2-dimethyl- 2.58 |
| $C_7H_8O_6$ C_7H_8S | Benzyl mercaptan 11.2 | | Cyclohexene, 2,3-dimethyl- 2.59 |
| ₩7××8₩ | | | Cyclooctene 2.83 |
| CITA | Sulfide, methyl phenyl 11.4 | | 2,4-Hexadiene, 2,5-dimethyl- 2.90 |
| C_7H_9N | Aniline, N-methyl- 7.3 | OH NO. | • |
| | Benzylamine 6.8 | $C_8H_{14}NiO_2S_4$ | Nickel(II), bis(2-propylcarbonothioyl-S,S')- 10.6 |
| $C_7H_{11}OT$ | 4H-Pyran-2-t, 2,3-dihydro-4,4-dimethyl- 15.17 | $C_8H_{14}O$ | Ethanol, 2-cyclohexylidene- 79F137 |
| | 4H-Pyran-3-t, 2,3-dihydro-4,4-dimethyl- 15.18 | $C_8H_{14}O_2S_2$ | Lipoic acid 11.45 |
| | | | |

| C_8H_{16} | 2-Pentene, 2,3,4-trimethyl- 2.48 | | α -Phellandrene 2.93 |
|--|--|-----------------------------------|---|
| | 2-Pentene, 2,4,4-trimethyl- 2.49 | | α-Pinene 2.74 |
| $C_8H_{16}O_3$ | Ethene, 1,1,2-triethoxy- 2.9 | | β-Pinene 2.75 |
| C_8H_{18} | Heptane, 3-methyl- 15.9 | | Propene, 1,1-dicyclopropyl-2-methyl- 2.25 |
| | Heptane, 4-methyl- 15.10 | | α-Terpinene 2.92 |
| | Pentane, 2,2,4-trimethyl- 1a.6 | | Terpinolene 2.61 |
| $C_8H_{18}S$ | Sulfide, dibutyl 11.20 | $C_{10}H_{16}N_2$. | p-Phenylenediamine, N,N,N',N'-tetramethyl- 7.19 |
| | Sulfide, di-(2-butyl) 11.21 | | Nickel(II), bis(4-imino-2-pentanonato-N,O)- 10.53 |
| | Sulfide, di-(2-methyl-2-propyl) 11.22 | $C_{10}H_{16}OSi$ | Norborna-2,5-diene, 2-(trimethylsiloxy)- 2.95 |
| $C_8H_{19}NO_2$ | 2-Propylamine, N,N-di(2-hydroxyethyl)-2-methyl- | $C_{10}H_{18}$ | Carvomethene 2.60 |
| | 6.29 | | 2,6-Octadiene, 2,6-dimethyl- (cis) 2.102 |
| $C_8H_{20}NiO_4P_2S$ | Nickel(II), bis(O,O'-diethyldithiophosphato-S,S')- 10.24 | | 2,6-Octadiene, 2,6-dimethyl- (trans) 2.103 |
| C_9H_7N | Quinoline 5.47 | | 2,6-Octadiene, 2,7-dimethyl- 2.105 |
| C_9H_8 | Indene 3.40 | $C_{10}H_{18}NiO_6$ | Nickel(II), diaquabis(2,4-pentanedionato-0,0')- 10.62 |
| C_9H_8N | Indole, 3-methyl- 79A106 | $C_{10}H_{18}O$ | Ethanol, 2-cyclooctylidene- 79F137 |
| $C_9H_8N_2O$ | Phenol, 4-(1-imidazolyl)- 79F268 | | 1,6-Octadiene-2-ol, 3,7-dimethyl- 2.101 |
| C_9H_{10} | Styrene, β -methyl- (cis) 3.7 | | 2,7-Octadien-1-ol, 3,7-dimethyl- 79F137 |
| | Styrene, β -methyl- (trans) 3.8 | $C_{10}H_{18}OSi$ | Norborn-2-ene, 2-(trimethylsiloxy)- 2.65 |
| $C_9H_{10}N_2$ | Aniline, p -cyano- N , N -dimethyl- 7.10 | $C_{10}H_{18}O_{2}$ | 2,6-Octadiene, 2,6-dimethyl-, mixture of hydroperoxides |
| $C_9H_{11}NO$ | Benzaldehyde, p -(N , N -dimethylamino)- 7.11 | 2 | obtained from its photosensitized oxygenation. 2.104 |
| $C_9H_{11}NO_3$ | Tyrosine 8.5 79A112 | | 2,5-Octadiene, 7-hydroperoxy-2,7-dimethyl- 2.100 |
| $C_9H_{11}NO_4$ | Alanine, 3–(3,4–dihydroxyphenyl)– 79F314 79F315 | | 2,7-Octadiene, 6-hydroperoxy-2,7-dimethyl- 2.106 |
| $C_9H_{12}O_3$ | Benzene, 1,2,3-trimethoxy- 3.29 | $C_{10}H_{20}N_2NiS_4$ | |
| | Benzene, 1,2,4-trimethoxy- 3.30 | $C_{10}H_{20}O$ | 2-Octen-1-ol, 3,4-dimethyl- 79F137 |
| | Benzene, 1,3,5-trimethoxy- 3.31 | 2 | 6-Octen-1-ol, 3,7-dimethyl- 2.82 |
| $C_9H_{13}N$ | Aniline, p -methyl- N , N -dimethyl- 7.9 | $C_{10}H_{20}O_4$ | Ethene, 1,1,2,2-tetraethoxy- 2.12 |
| | Propylamine, 3-phenyl- 6.10 | $C_{10}H_{21}NO$ | Piperidine, 4-hydroxy-1,2,2,6,6-pentamethyl- 6.33 |
| $C_9H_{13}NO$ | Aniline, m -methoxy- N , N -dimethyl- 7.12 | $C_{10}H_{24}NiO_4P_2S$ | S ₄ Nickel(II), bis(O,O'-di-2-propyldithiophosphato-S,S')- |
| | Aniline, p-methoxy-N,N-dimethyl- 7.13 | | 10.25 |
| $C_9H_{13}N_3O_5$ | Cytidine 14.40 | $C_{11}H_8O_2$ | 1,4-Naphthalendione, 2-methyl- 3.42 |
| C_9H_{14} | Cyclobutane, (1-cyclopropylethylidene)- 2.27 | $C_{11}H_{10}Cl_2N_2O_2$ | |
| | Propene, 1,1-dicyclopropyl- 2.24 | | 2,3-dioxide, 1,4-dichloro- 13.11 |
| C_9H_{16} | Cyclooctene, 1-methyl- 2.84 | $C_{11}H_{10}O$ | Furan, 2-(4'-methylphenyl)- 5.24 |
| C_9H_{18} | 1-Nonene 2.85 | | Furan, 3-(4'-methylphenyl)- 5.25 |
| | 4-Octene, 4-methyl- (cis) 2.79 | $C_{11}H_{10}O_2$ | Furan, 2-(4'-methoxyphenyl)- 5.26 |
| | 4-Octene, 4-methyl- (trans) 2.78 | | Furan, 3-(4'-methoxyphenyl)- 5.27 |
| | 4-Octene, 4-methyl- 2.80 2.81 | | Furfuryl alcohol, α-phenyl- 5.11 |
| C ₉ H ₁₉ NO | Piperidine, 4–hydroxy–2,2,6,6–tetramethyl– 6.18 | $C_{11}H_{12}N_2O_2$ | Tryptophan 8.8 79A112 |
| $C_{10}H_7BrO$ | Furan, 3-(4'-bromophenyl)- 5.23 | $C_{11}H_{13}Cl$ | Styrene, m -chloro- α,β,β -trimethyl- 3.11 |
| C ₁₀ H ₇ ClO | Furan, 2-(4'-chlorophenyl)- 5.22 | | Styrene, p -chloro- α, β, β -trimethyl- 3.12 |
| $C_{10}H_7FO$ | Furan, 3-(4'-fluorophenyl)- 5.21 | $C_{11}H_{14}$ | 2-Butene, 3-methyl-1-phenyl- 3.9 |
| $C_{10}H_8O$ | Furan, 2-phenyl- 5.19 | | Styrene, α,β,β -trimethyl- 3.10 |
| | Furan, 3-phenyl- 5.20 | $C_{11}H_{16}$ | Cyclobutane, (dicyclopropylmethylidene)— 2.19 |
| | α-Naphthol 4.29 | | Ethene, 1,1,2-tricyclopropyl- 2.10 |
| | β -Naphthol 4.30 | | Nopadiene 2.98 |
| $C_{10}H_9N$ | Naphthalene, 2-amino- 7.2 | $C_{11}H_{16}O_5$ | Benzene, pentamethoxy- 3.37 |
| $C_{10}H_{10}D_6$ | Propene- d_6 , 1,1-dicyclopropyl-2-methyl- 2.26 | $C_{11}H_{16}S$ | Sulfide, methyl 4–(2–methyl–2–propyl)phenyl 11.13 |
| $C_{10}H_{10}Fe$ | Ferrocene 10.123 | $C_{11}H_{21}N$ | Piperidine, 1-cyclohexyl- 6.36 |
| $C_{10}H_{10}N$ | Indole, 2,3-dimethyl- 79A106 | $C_{11}H_{23}NO$ | Piperidine, N-(2-hydroxyethyl)-2,2,6,6-tetramethyl- |
| $C_{10}H_{12}O$ | Anethole 3.28 | * | 6.34 |
| $C_{10}H_{12}O_5$ | Furan, 3,4-diethoxycarbonyl- 5.32 | $C_{11}H_{26}N_2$ | Diethylamine, N-(7-aminoheptyl)- 6.27 |
| $C_{10}H_{13}N_5O_4$ | Adenosine 14.38 | C ₁₂ H ₉ NO | Phenoxazine 5.52 |
| $C_{10}H_{13}N_5O_5$ | Guanosine 14.36 | $C_{12}H_9NS$ | Phenothiazine 11.36 |
| $C_{10}H_{14}$ | Cyclopropane, (dicyclopropylmethylidene)- 2.18 | $C_{12}H_{10}S$ | Sulfide, diphenyl 11.23 |
| $C_{10}H_{14}C_0O_4$ | Cobalt(II), bis(2,4-pentanedionato-0,0')- 10.54 | $C_{12}H_{11}N$ | Diphenylamine 7.4 |
| $\mathrm{C_{10}H_{14}CuO_{4}}$ | Copper(II), bis(2,4-pentanedionato-0,0')- 10.56 | $C_{12}H_{12}$ | Naphthalene, 1,4-dimethyl- 3.41 |
| $C_{10}H_{14}N_2$ | Nicotine 6.30 | $C_{12}H_{12}N_2$ | Biphenyl, 4,4'-diamino- 7.15 |
| C ₁₀ H ₁₄ NiO ₄ | Nickel(II), bis(2,4-pentanedionato-0,0')- 10.55 | $C_{12}H_{12}O_2$ | [2.2](2,5)Furanophane 5.34 |
| $C_{10}H_{14}NiS_4$ | Nickel(II), bis(2,4-pentanedithionato-S,S')- 10.64 | | Furfuryl alcohol, α-benzyl- 5.12 |
| $C_{10}H_{14}O_4$ | Benzene, 1,2,3,4-tetramethoxy- 3.32 | $C_{12}H_{13}N$ | Styrene, m -cyano- α, β, β -trimethyl- 3.15 |
| | Benzene, 1,2,3,5-tetramethoxy- 3.33 | ** ** | Styrene, p -cyano- α, β, β -trimethyl- 3.16 |
| | Benzene, 1,2,4,5-tetramethoxy- 3.34 | $(C_{12}H_{15}N)_n$ | Permanax 45 5.48 |
| $C_{10}H_{14}O_4Zn$ | Zinc(II), bis(2,4-pentanedionato-0,0')- 10.57 | $C_{12}H_{16}$ | Styrene, m -methyl- α, β, β -trimethyl- 3.14 |
| $C_{10}H_{15}N$ | Butylamine, 4-phenyl- 6.11 | 0.11.0 | Styrene, p -methyl- α, β, β -trimethyl- 3.13 |
| $C_{10}H_{16}$ | Alloocimine-A 2.116 | $C_{12}H_{16}O$ | Styrene, m -methoxy- α, β, β -trimethyl- 3.17 |
| | Δ^2 -Carene 2.68 | a | Styrene, p -methoxy- α, β, β -trimethyl- 3.18 |
| | Δ^3 -Carene 2.69 | $C_{12}H_{18}$ | Bicyclo[2.2.0]hexa-2,5-diene, hexamethyl- 2.99 |
| | Δ^4 -Carene 2.70 | 0.44.6 | Cyclopentane, (dicyclopropylmethylidene)- 2.20 |
| | Limonene 2.97 | $C_{12}H_{18}O$ | Cyclohexanone, 2-cyclohexylidene- 2.15 |
| | Norbornane, 7,7-dimethyl-2-methylidene- 2.75a | $C_{12}H_{18}O_2$ | Durohydroquinone monoethyl ether 4.24 |
| | Norborn-2-ene, 2,7,7-trimethyl- 2.66 | $C_{12}H_{18}O_6$ | Benzene, hexamethoxy- 3.39 |
| | $\Delta^{9,10}$ -Octalin 2.16 | $C_{12}H_{20}$ | Cyclohexane, cyclohexylidene- 2.13 |
| | | | |

| $C_{12}H_{20}O$ | Cyclohexanol, 2-cyclohexylidene- 2.14 Furan, 2,5-di(2-methyl-2-propyl)- 79A106 | $\mathrm{C_{14}H_{28}N_2NiS_4}$ | Nickel(II), bis(N,N-di-2-propyldithiocarbamato-S,S')-10.12 |
|--|--|---------------------------------|--|
| $\mathrm{C_{12}H_{20}OS}i$ | Norborna-2,5-diene, 7,7-dimethyl-2-(trimethylsiloxy)-2.96 | $\mathrm{C_{14}H_{28}N_2S_4Zn}$ | |
| $C_{12}H_{22}OSi$ | Norborn-2-ene, 7,7-dimethyl-2-(trimethylsiloxy)- 2.67 | $C_{15}H_{10}S_3$ | 1,3-Dithiole-2-thione, 4,5-diphenyl- 11.46 |
| $C_{12}H_{27}N$ | Tributylamine 6.28 | $C_{15}H_{11}NO$ | Oxazole, 2,5-diphenyl- 5.51 |
| $C_{12}H_{27}PO_3$ | Phosphite, tributyl- 15.25 | $C_{15}H_{12}$ | Anthracene, 9-methyl- 3.47 |
| $C_{13}H_8N_2$ | 9-Diazofluorene 9.6 | $C_{15}H_{12}N$ | Indole, 3-methyl-2-phenyl- 79A106 |
| $C_{13}H_8O_2N_2$ | Diazomethane, di(4-chlorophenyl) 9.4 | $C_{15}H_{12}O$ | Anthracene, 9-methoxy- 3.48 |
| $C_{13}H_9BrN_2$ | Diazomethane, (4-bromophenyl)phenyl 9.2 | $C_{15}H_{14}$ | Stilbene, \alpha-methyl-(cis) 3.22 |
| $C_{13}H_{10}NO^{-}$ | Benzophenone oximate anion 13.2 | | Stilbene, a-methyl-(trans) 3.23 |
| $C_{13}H_{10}N_2$ | Diazomethane, diphenyl 9.1 | $C_{15}H_{14}N_2$ | Diazomethane, di(4-methylphenyl) 9.5 |
| $C_{13}H_{11}NO$ | Benzophenone oxime 13.3 | $C_{15}H_{18}N_2$ | Benzene, 1-(2-propylamino)-4-phenylamino- 7.16 |
| $C_{13}H_{11}NS$ | Phenothiazine, 10-methyl- 11.37 | $C_{15}H_{21}C_0O_6$ | Cobalt(III), tris(2,4-pentanedionato-0,0')- 10.61 |
| $C_{13}H_{14}O_2$ | Furfuryl alcohol, α-phenethyl- 5.13 | $C_{15}H_{21}CrO_6$ | Chromium(III), tris(2,4-pentanedionato-O,O')- 10.58 |
| $C_{13}H_{16}$ | Styrene, α -cyclopropyl- β , β -dimethyl- 3.20 | $C_{15}H_{21}FeO_6$ | Iron(III), tris(2,4-pentanedionato-0,0')- 10.60 |
| $C_{13}H_{16}N_2O$ | Dipyrromethene, 5'-oxo-4-ethyl-3,5-dimethyl-1',5'- | $C_{15}H_{21}MnO_6$ | Manganese(III), tris(2,4-pentanedionato-0,0')- 10.59 |
| | dihydro-(2.2')- 14.22 79A113 | $C_{15}H_{24}$ | Caryophyllene (-) 2.111 |
| | Dipyrromethene, 5'-oxo-3'-ethyl-4',5'-dimethyl-1',5'- | $C_{15}H_{24}O$ | Phenol, 4-methyl-2,6-di(2-methyl-2-propyl)- 4.7 |
| | dihydro-(2.2')- 79A113 | $C_{15}H_{24}O_2$ | Benzyl alcohol, 4-hydroxy-3,5-di(2-methyl-2-butyl)- |
| | Dipyrromethene, 5'-oxo-4-ethyl-3,5-dimethyl-1',5'- | | 4.9 |
| | dihydro-(2.2')- 79A113 | | Phenol, 3-methoxy-4,6-di(2-methyl-2-propyl)- 4.16 |
| $C_{13}H_{16}O_2$ | Benzonorbornene, 1,4-dimethoxy- 3.39a | | Phenol, 4-methoxy-2,6-di(2-methyl-2-propyl)4.8 |
| $C_{13}H_{19}N$ | Styrene, p -(N , N -dimethylamino)- α , β , β , 3.19 | $C_{16}H_{10}Cl_2O$ | Furan, 2,5-di(4-chlorophenyl)- 79A106 |
| $C_{13}H_{24}$ | 1,6-Decadiene, 2,6,9-trimethyl- (cis) 2.108 | $C_{16}H_{12}N_4O$ | 2-Pyrazolin-5-one, 4-(4'-aminophenyl)imino-3-methyl- |
| | 1,6-Decadiene, 2,6,9-trimethyl- (trans) 2.107 | | 1-phenyl- 9.16 |
| | 1,6-Undecadiene, 2,6-dimethyl- (cis) 2.110 | $C_{16}H_{12}O$ | Furan, 2,3-diphenyl- 79A106 |
| | 1,6-Undecadiene, 2,6-dimethyl- (trans) 2.109 | | Furan, 2,5-diphenyl- 5.30 79A106 |
| $C_{13}H_{25}NO_2$ | Piperidine, N-(2-acetoxyethyl)-2,2,6,6-tetramethyl- 6.35 | | Furan, 3,4-diphenyl- 5.31 |
| $C_{14}H_8Cl_2$ | Anthracene, 9,10-dichloro- 3.52 | $C_{16}H_{14}$ | Anthracene, 9,10-dimethyl- 3.53 79F148 |
| $C_{14}H_8O_6S_2^{2-}$ | 1,5-Anthracenedisulfonate ion 3.55 | $C_{16}H_{14}CoN_2O_2$ | Cobalt(II), 2,2'-[1,2-ethanediylbis- |
| C ₁₄ H ₉ Cl | Anthracene, 1-chloro- 3.45 | | (nitrilomethylidyne)]bis[phenolato(2-)- N , N ', O , O ']- 10.92 |
| | Anthracene, 9-chloro- 3.46 | $C_{16}H_{14}N_2NiO_2$ | Nickel(II), 2,2'-[1,2-ethanediylbis- |
| $C_{14}H_9O_3S^2$ | 1-Anthracenesulfonate ion 3.49 | | (nitrilomethylidyne)]bis[phenolato(2-)-N,N',O,O']- 10.93 |
| | 2-Anthracenesulfonate ion 3.50 | $C_{16}H_{14}O_2$ | Anthracene, 9,10-dimethoxy- 3.54 |
| $C_{14}H_{10}$ | Anthracene 3.44 | 0.11 | 3,6-Dioxacyclohexene, 1,2-diphenyl- 2.63 |
| C ₁₄ H ₁₂ | Stilbene (cis) 3.21 | C ₁₆ H ₁₆ | 2-Butene, 2,3-diphenyl- 79F051 |
| C ₁₄ H ₁₂ Br ₂ NiO ₆ | Nickel(II), diaquabis(5-bromo-2-hydroxy- | $C_{16}H_{16}CIN_3O$ | 1,2,3-Benzo[2 <i>H</i>]triazole, 2-[3'-chloro-2'-hydroxy-5'- |
| | benzaldehydato-0,0')- 10.66 | C II N NO | (2-methyl-2-propyl)phenyl]- 4.19 |
| | Nickel(II), bis[2-iminomethylphenolato-N,O]- 10.76 | $C_{16}H_{16}N_2NiO_4$ | |
| $C_{14}H_{12}N_2N_1O_4$ | Nickel(II), bis(2-hydroxybenzaldehyde oximato-N,O)- | C II N N:S | 10.72 Nickel(II) kief N (n. methylphenyl)dithiogerhemete S S'1 |
| C II N NIC | 10.71 | $C_{16}H_{16}N_2NiS_4$ | Nickel(II), bis[N -(p -methylphenyl)dithiocarbamato- S - S ']- 10.21 |
| $C_{14}H_{12}N_2NiS_4$ | Nickel(II), bis(N-phenyldithiocarbamato-S,S')- 10.7 | $C_{16}H_{16}O_2$ | Stilbene, 1,2-dimethoxy- 3.24 |
| CHNO | Diazomethane, (4-methoxyphenyl)phenyl 9.3 | $C_{16}H_{18}NiO_3S$ | Nickel(II), aqua[2,2'-thiobis-(3,4-dimethyl)-phenolato- |
| $C_{14}H_{12}N_2O$ | Benzophenone oxime, O-methyl ether 13.4 | C161118141O35 | 0.00]- 10.99 |
| C ₁₄ H ₁₃ NO | Nickel(II), diaquabis(2-hydroxybenzaldehydato-0,0')- | $C_{16}H_{18}NiO_8$ | Nickel(II), diaquabis(2-hydroxy-5-methoxy- |
| $C_{14}H_{14}NiO_6$ | 10.65 | C161118111O8 | benzaldehydato- O,O')- 10.67 |
| сиѕ | Sulfide, dibenzyl 11.24 | $C_{16}H_{20}N_2O$ | [2.2']-Dipyrromethene, 5'-oxo-4'-vinyl-4-ethyl-3',3,5- |
| $C_{14}H_{14}S$ $C_{14}H_{16}O_2$ | Furfuryl alcohol, α-(3-phenylpropyl)- 5.14 | 01611201120 | trimethyl-1',5'-dihydro- 14.17 79A113 |
| $C_{14}H_{16}O_2$ $C_{14}H_{18}N_2O$ | [2.2']-Dipyrromethene, 5'-oxo-3',4'-diethyl-5-methyl- | $C_{16}H_{24}O_{2}$ | Phenol, 4-acetyl-2,6-di(2-methyl-2-propyl)- 4.10 |
| 01411181720 | 1',5'-dihydro- 14.21 | $C_{16}H_{24}O_3$ | Benzoic acid, 4-hydroxy-3,5-di(2-methyl-2-propyl)-, |
| | [2.2']-Dipyrromethene, 5'-oxo-3'-ethyl-4',3,5-trimethyl- | 10 24 3 | methyl ester 4.11 |
| | 1',5'-dihydro- 14.19 | $C_{16}H_{26}O$ | Anisole, 2,6-di-t-butyl-4-methyl- 3.36 |
| | [2.2']-Dipyrromethene, 5'-oxo-4',4,5-trimethyl-3'-ethyl- | $C_{16}H_{26}O_2$ | Benzene, 1,3-dimethoxy-4,6-di-t-butyl- 3.35 |
| | 1',5'-dihydro- 14.20 | $C_{16}H_{34}$ | Hexadecane 1a.7 |
| $C_{14}H_{19}NO_3S$ | L-Methionine, CBZ-, methyl ester 8.3 | $C_{17}H_{12}OS$ | 4H-Pyran-4-thione, 2,6-diphenyl- 11.34 |
| $C_{14}H_{21}BrO$ | Phenol, 4-bromo-2,6-di(2-methyl-2-propyl)- 4.5 | $C_{17}H_{12}S_2$ | 4H-Thiopyran-4-thione, 2,6-diphenyl- 11.44 |
| $C_{14}H_{21}CIO$ | Phenol, 4-chloro-2,6-di(2-methyl-2-propyl)- 4.6 | $C_{17}H_{14}O_2$ | Furfuryl alcohol, α,α-diphenyl- 5.16 |
| $C_{14}H_{22}O$ | Phenol, 2,6-di(2-methyl-2-propyl)- 4.1 | $C_{17}H_{15}N_3O_2$ | 2-Pyrazolin-5-one, 4-(4'-methoxyphenyl)-imino-3- |
| $C_{14}H_{26}$ | 4,8-Dodecadiene, 4,8-dimethyl-(trans,trans)- 2.112 | | methyl-1-phenyl- 9.28 |
| | 4,8-Dodecadiene, 4,8-dimethyl- 2.113 | $C_{17}H_{19}CIN_2S$ | Chloropromazine 11.38 |
| $C_{14}H_{26}O$ | Ethanol, 2-cyclododecylidene- 79F137 | $C_{17}H_{22}N_2$ | Dipyrromethene, 4,4'-diethyl-3,5,3',5'-tetramethyl- |
| $C_{14}H_{26}O_2$ | 4,8-Dodecadiene, 4,8-dimethyl-, mixture of | 017**22**2 | (2.2')- 79F118 |
| | hydroperoxides obtained from its photosensitized | сим | Dipyrromethane, 4,4'-diethyl-3,5,3',5'-tetramethyl- |
| | oxygenation. 2.114 | $C_{17}H_{24}N_2$ | (2.2')- 79F118 |
| $C_{14}H_{28}CoN_2S_4$ | Cobalt(II), $bis(N,N-di-2-propyldithiocarbamato-S,S')$ - | CHNO | • |
| | 10.11 | $C_{17}H_{24}N_2O$ | [2.2']-Dipyrromethene, 5'-oxo-3',4',4-triethyl-3,5- |
| $\rm C_{14}H_{28}CuN_{2}S_{4}$ | Copper(II), $bis(N,N-di-2-propyldithiocarbamato-S,S')$ - | | dimethyl-1',5'-dihydro- 14.18 79A113 |
| | 10.13 | $C_{17}H_{24}N_4NiO_6$ | Nickel(II), (3,11-bisacetyl-4,10-dimethyl-1,5,9,13- |
| $C_{14}H_{28}MnN_2S_4$ | Manganese(II), bis(N,N-di-2-propyldithiocarbamato-S,S')- | | tetraazacyclopentadeca-1,3,9,11-tetraene-N,N',N'',N''')- |
| | 10.10 | | 10.116 |

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|--|--|--|--|
| $C_{17}H_{26}O_3$ | Propanoic acid, 4-hydroxy-3,5-di(2-methyl-2-propyl)- | $C_{21}H_{32}O_2$ | Pregnenolone 14.12 |
| | phenyl ester 4.23 | $C_{21}^{21}H_{34}^{32}O_{2}$ | Arachidonic acid, methyl ester 14.8 |
| $C_{18}H_{12}$ | 1,2-Benzanthracene 3.60 | $C_{21}H_{42}FeN_3S_6$ | Iron(III), tris(N,N-di-2-propyldithiocarbamato-S,S')- |
| | Naphthacene 3.62 | | 10.15 |
| $C_{18}H_{12}O$ | Benzo[b]cyclopentadieno[e]pyran, 2-phenyl- 5.40 | $C_{22}H_{14}$ | 1,2,5,6-Dibenzanthracene 3.64 |
| C ₁₈ H ₁₅ P | Phosphine, triphenyl- 15.27 | C II N C | Pentacene 3.65 |
| C ₁₈ H ₁₆ O | 2-Penten-1-ol, 3,4,4-trimethyl- 79F137 | $C_{22}H_{16}N_2O$ | Aniline, 4-(2',3'-benzo-4'- |
| $C_{18}H_{16}O_2$ $C_{18}H_{18}N_2NiO_2$ | Furfuryl alcohol, α-benzhydryl- 5.15 Nickel(II), 2,2'-[1,2-ethanediylbis- | $C_{22}H_{18}O$ | oxocyclohexadienyliden)amino-N-phenyl- 9.31 Isobenzofuran, 5,6-dimethyl-1,3-diphenyl- 5.37 |
| 018111811211102 | (nitriloethylidyne)]bis[phenolato(2-)- N , N ', O , O ']- 10.94 | C ₂₂ H ₁₈ O C ₂₂ H ₂₆ Br ₂ N ₂ Ni | |
| $C_{18}H_{18}N_4O$ | 2-Pyrazolin-5-one, 4-(4'-dimethylamino-phenyl)imino- | 0221126012112111 | Nickel(II), bis[4-bromo-2-[(butylimino)methyl]- |
| | 3-methyl-1-phenyl- 9.18 | • | phenolato-N,O]- 10.80 |
| $C_{18}H_{20}B_2N_{12}N_1$ | Nickel(II), bis[hydrotris(1-pyrazolato)borato]- 10.5 | $C_{22}H_{26}N_4O$ | 2-Pyrazolin-5-one, 4-(4'-diethylamino-2',6'- |
| $C_{18}H_{20}N_2NiO_4$ | Nickel(II), bis(2-hydroxy-4-methylacetophenone | | dimethylphenyl)-imino-3-methyl-1-phenyl- 9.23 |
| 0 11 11110 0 | oximato-N,O)- 10.73 | | 2-Pyrazolin-5-one, 4-(4'-dimethylamino-2',3',5',6'- |
| $C_{18}H_{21}NNiO_2S$ | | | tetramethylphenyl)imino-3-methyl-1-phenyl- 9.20 |
| СИМ | dimethyl)phenolato- O,O']- 10.102 | $C_{22}H_{27}NNiO_2S$ | |
| ${ m C_{18}H_{22}N_2} \ { m C_{18}H_{22}N_4Ni}$ | Benzene, 1-cyclohexylamino-4-phenylamino- 7.17 Nickel(II), bis(1-methylamino-2- | C H N N'O | dimethyl)phenolato-0,0']- 10.108 |
| 0181122114111 | methyliminocycloheptatriene-N,N')- 10.46 | $C_{22}H_{28}N_2NiO_2$ | Nickel(II), bis[2-[(butylimino)methyl]phenolato- N , O]- 10.79 |
| $C_{18}H_{23}ClN_2$ | Benzene, 1-cyclohexylamino-4-phenylamino-, | | Nickel(II), bis[2-[(1-methylpropylimino)methyl]- |
| 10 23 2 | hydrochloride 7.18 | | phenolato- N,O]- 10.82 |
| $C_{18}H_{30}O$ | Phenol, 2,4,6-tri(2-methyl-2-propyl)- 4.12 | | Nickel(II), bis[2-[(2-methyl-2-propylimino)methyl]- |
| $C_{18}H_{30}O_2$ | Phenol, 4-(2-methyl-2-propoxy)-2,6-di(2-methyl-2- | | phenolato-N,O]- 10.83 |
| | propyl)- 4.13 | $C_{22}H_{29}N_3O$ | 1,2,3-benzo[2H]triazole, 2-[2'-hydroxy-3',5'-di(2- |
| $C_{18}H_{33}PO_3$ | Phosphite, tricyclohexyl- 15.26 | | methyl-2-butyl)- phenyl]- 4.21 |
| C ₁₈ H ₃₆ CoN ₂ S ₄ | Cobalt(II), bis(N,N-dibutyldithiocarbamato-S,S')- 10.16 | $C_{22}H_{32}O_2$ | Retinyl acetate 79F463 |
| CH NNS | Copper(II), bis(N,N-dibutyldithiocarbamato-S,S')- 10.18 | $C_{23}H_{21}IN_2S_2$ | 2,2'-Thiacarbocyanine, 3,8,3',10-di(1,3-propanediyl)-, |
| $C_{18}H_{36}N_2NiS_4$ $C_{18}H_{36}N_2S_4Zn$ | Nickel(II), bis(N,N -dibutyldithiocarbamato- S,S')- 10.17 Zine(II), bis(N,N -dibutyldithiocarbamato- S,S')- 10.19 | C H D-CIN | iodide 9.51 |
| $C_{19}H_{13}O_2S^-$ | Fluoren-9-yl anion, 9-benzenesulfonyl 11.47 | C ₂₃ 11 ₂₃ DfCl ₂ (\(\frac{1}{2}\) | S ₂ 2,2'-Thiacarbocyanine, 5,5'-dichloro-3,9,3'-triethyl-, bromide 9.44 |
| $C_{19}H_{22}N_2O_3$ | Dregamine 6.31 | $C_{23}H_{23}IN_2S_2$ | 2,2'-Thiadicarbocyanine, 3,3'-diethyl-, iodide 9.52 |
| $C_{19}H_{32}O_2$ | Linolenic acid, methyl ester 14.7 | $C_{23}H_{25}BrN_2S_2$ | |
| $C_{19}H_{34}O_{2}$ | Linoleic acid, methyl ester 14.6 | $C_{23}^{23}H_{29}^{23}N_3O_2$ | Aniline, N,N-diethyl-4~[N-(phenylaminocarbonyl)- |
| $C_{19}H_{36}O_2$ | Oleic acid, methyl ester 14.5 | 20 20 2 | pivaloylmethylene]amino- 9.10 |
| $C_{19}H_{38}O_2$ | Stearic acid, methyl ester 14.4 | $C_{23}H_{32}O_3$ | 16-Dehydropregnenolone-3-acetate 14.15 |
| $C_{20}H_{14}$ | Anthracene, 9-phenyl- 3.51 | $C_{23}H_{36}N_2O_2$ | Aniline, $4-(N-dipival oylmethylene)$ amino $-3,N,N-$ |
| $C_{20}H_{14}N_2NiO_2$ | Nickel(II), 2,2'-[1,2-phenylenebis- | | triethyl- 9.7 |
| CHO | (nitrilomethylidyne)]bis[phenolato(2-)-N,N',O,O']- 10.96 | $C_{24}H_{16}N_2NiO_2$ | |
| $C_{20}H_{14}O$ | Isobenzofuran, 1,3-diphenyl- 5.36 79A106 79E106 79E611 79E463 79N020 79N041 | CHO | methylidyne)]bis[phenolato(2-)- N , N' , O , O']- 10.97 |
| C ₂₀ H ₁₆ | 1,2-Benzanthracene, 9,10-dimethyl- 3.61 | $C_{24}H_{18}O \ C_{24}H_{20}$ | Phenol, 2,4,6-triphenyl- 4.22 2-Butene, 2,3-di(α-naphthyl)- 79F051 |
| $C_{20}H_{16}$ $C_{20}H_{22}N_4O$ | 2-Pyrazolin-5-one, 4-(4'-amino-2',3',5',6'- | $C_{24}H_{20}$ $C_{24}H_{20}$ | 2-Butene, 2,3-di(β -naphthyl)- 79F051 |
| -2022- 4- | tetramethylphenyl)imino-3-methyl-1-phenyl- 9.17 | | S_4 Cobalt(II), bis $(O,O'$ -diphenyldithiophosphato- S,S')- |
| | 2-Pyrazolin-5-one, 4-(4'-diethylaminophenyl)imino-3- | 24 20 4 2 | 10.28 |
| | methyl-1-phenyl- 9.21 | $C_{24}H_{20}CrO_4P_2S$ | S_4 Chromium(II), bis(O,O' -diphenyldithiophosphato- S,S')- |
| | 2-Pyrazolin-5-one, 4-(4'-dimethylamino-3',5'- | | 10.32 |
| | dimethylphenyl)imino-3-methyl-1-phenyl- 9.19 | $C_{24}H_{20}CuO_4P_2$ | |
| $C_{20}H_{24}CIN_3O$ | 1,2,3-benzo[2 <i>H</i>]triazole, 2-[2'-hydroxy-3',5'-di(2- | : 0 H 340 D | 10.30 |
| C H N N'O | methyl-2- propyl)phenyl]-5-chloro- 4.20 | $C_{24}H_{20}NiO_4P_2S$ | |
| $C_{20}H_{24}N_2NiO_2$ | Nickel(II), bis[2-[(2-propylimino)methyl]phenolato- N,O]- 10.78 | СНОРРЫ | 10.29 S_4 Lead(II), bis(O,O' -diphenyldithiophosphato- S,S')- 10.33 |
| C ₂₀ H ₂₅ NNiO ₂ S | | | In Zinc(II), bis(0,0'-diphenyldithiophosphato-S,S')- 10.31 |
| ~20×125-1111020 | phenolato- $0.0'$]- 10.106 | C ₂₄ H ₂₅ IN ₂ S ₂ | 2,2'-Thiacarbocyanine, 3,3'-diethyl-8,9-(1,3- |
| $C_{20}H_{26}N_2O$ | Aniline, N,N -diethyl-3,5-dimethyl-4- $(4'-oxo-2',6'-$ | 24 252-2 | propanediyl)-, iodide 9.50 |
| 20 20 2 | dimethylcyclohexadienyliden)amino- 9.30 | $C_{24}H_{30}N_4O$ | 2-Pyrazolin-5-one, 4-(4'-diethylamino-2'- |
| $C_{20}H_{26}O$ | Phenol, 2,6-di(2-methyl-2-propyl)-4-phenyl- 4.14 | | methylphenyl)imino-3-(2-methyl-2-propyl)-1-phenyl- |
| $C_{20}H_{28}$ | Adamantane, adamantylidene- 2.17 | | 9.24 |
| $C_{20}H_{28}O$ | 11-cis-Retinal 79F463 | $C_{24}H_{31}N_3O_2$ | Aniline, N,N-diethyl-3-methyl-4-[N-(phenylamino- |
| | 13-cis-Retinal 79F463 | | carbonyl)pivaloylmethylene]amino- 9.11 |
| | Retinal (all trans) 79F463 | $C_{24}H_{32}N_2NiO_4$ | |
| $C_{20}H_{30}O$ | Retinol (all trans) 2.119 | C H C O D | phenolato-N,0]- 10.81 |
| C ₂₁ H ₁₉ BrCl ₂ N ₂ | S ₂ 2,2'-Thiacarbocyanine, 5,5'-dichloro-3,3'-diethyl-, bromíde 9.39 | $C_{24}H_{44}C0U_4P_2$ | S_4 Cobalt(II), bis(O,O' -dicyclohexyldithiophosphato- S,S')- 10.26 |
| CHIN | 2,2'-Cyanine, 1,1'-diethyl-, iodide 9.34 | $C_{24}H_{44}NiP_2S_4$ | Nickel(II), bis(dicyclohexyldithiophosphinato-S,S')- |
| $C_{21}H_{23}IN_2 C_{21}H_{24}N_4O$ | 2-Pyrazolin-5-one, 4-(4'-diethylamino-2'- | 02411441111 204 | 10.27 |
| G214124114U | methylphenyl)imino-3-methyl-1-phenyl- 9.22 | $C_{25}H_{19}N$ | 4-H-Cyclopentadieno[b]quinoline, 1,2-diphenyl-4- |
| $C_{21}H_{26}O_3$ | Benzophenone, 2-hydroxy-4-octyloxy- 4.3 | 20 19° | methyl- 5.46 |
| 21 20 3 | Salicylic acid, 4-(1,1,3,3-tetramethylbutyl)phenyl ester | $C_{25}H_{23}BF_4N_4S$ | |
| | 4.2 | | tetrafluoroborate 9.45 |
| $C_{21}H_{28}O$ | Phenol, 4-benzyl-2,6-di(2-methyl-2-propyl)- 4.15 | $\mathrm{C_{25}H_{25}ClN_2}$ | 2,2'-Carbocyanine, 1,1'-diethyl-, chloride 9.36 |
| $C_{21}H_{30}O_3$ | 7-Dehydroandrosterone-3-acetate 14.16 | $C_{25}H_{25}IN_2S_2$ | 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 | $C_{28}H_{42}O_2S$ | Phenol, 2,2'-thiobis[4-(1,1,3,3-tetramethyl-butyl)-4.32 |
|--|---|--|---|
| $C_{25}H_{26}N_4O_2$ | Aniline, 4-[N-di(phenylaminocarbonyl)methylene]- | C ₂₈ H ₄₃ N | Diphenylamine, 4,4'-di(1,1,3,3-tetramethylbutyl)- 7.5 |
| $C_{25}H_{32}N_4O$ | amino-N,N-diethyl- 9.15 2-Pyrazolin-5-one, 4-(4'-diethylamino-2',6'- | $C_{28}H_{43}NNiO_2S$ | Nickel(II), ammine[$2,2'$ -thiobis- 4 -($1,1,3,3$ -tetra-methylbutyl)phenolato- $0,0'$]- 10.100 |
| C ₂₅ 11 ₃₂ 11 ₄ O | dimethylphenyl)-imino-3-(2-methyl-2-propyl)-1- | $C_{28}H_{44}O$ | Ergosterol 14.11 |
| | phenyl- 9.25 | $C_{28}H_{48}O_2$ | β -Tocopherol 4.26 |
| $C_{25}H_{34}O_{3}$ | Benzophenone, 2-hydroxy-4-dodecyloxy- 4.4 | 25 45 2 | γ-Tocopherol 4.27 |
| $C_{26}H_{16}$ | 9,9'-Bifluorenylidene 3.43 | $C_{29}H_{20}O$ | Cyclopentadienone, tetraphenyl- 3.38 |
| $C_{26}H_{17}Cl$ | Anthracene, 1-chloro-9,10-diphenyl- 3.57 | $C_{29}H_{28}N_2O_3S_3$ | 2,2'-Thiacarbocyanine, 3,3'-diethyl-8,10-ethanediyl-, |
| C ₂₆ H ₁₈ | Anthracene, 9,10-diphenyl- 3.56 | CHNOC | toluenesulfonate 9.49 |
| $C_{26}H_{20}CoN_2O_2$ | Cobalt(II), bis[2-[(phenylimino)methyl]phenolato-N,O]- 10.85 | $C_{29}H_{30}N_2O_3S_3$ | 2,2'-Thiacarbocyanine, 3,3'-diethyl-8,10-dimethyl-, toluenesulfonate 9.47 |
| $C_{26}H_{20}CuN_2O_2$ | Copper(II), bis[2-{(phenylimino)methyl]phenolato-N,O}- 10.87 | $C_{29}H_{30}N_2O_5S_3$ | 2,2'-Thiacarbocyanine, 3,3'-diethyl-5,5'-dimethoxy-, toluenesulfonate 9.38 |
| $\mathrm{C_{26}H_{20}N_2NiO_2}$ | Nickel(II), bis[2-[(phenylimino)methyl]phenolato-N,O]- 10.86 | $C_{29}H_{42}O_3$ | Benzoic acid, 4-hydroxy-3,5-di(2-methyl-2-propyl)-, 2',4'-di(2-methyl-2-propyl)phenyl ester 4.18 |
| $\mathrm{C_{26}H_{20}N_2NiS_4}$ | Nickel(II), bis $(N,N-diphenyldithiocarbamato-S,S')$ - | $-C_{29}H_{50}O_{2}$ | α -Tocopherol 4.28 |
| 2620210-4 | 10.20 | $C_{30}H_{24}Cl_2N_6Ru$ | • |
| $\mathrm{C_{26}H_{22}N_4NiO_2}$ | Nickel(II), bis[2-[(4-aminophenylimino)methyl]- | $C_{30}H_{28}N_6O_2$ | 2-Pyrazolin-5-one, 4,4'-[2,3,5,6-tetramethyl- |
| | phenolato-N,O]- 10.91 | | phenylenebis]-3-methyl-1-phenyl- 9.29 |
| | Nickel(II), bis[2-(phenylaminoimino)methylphenolato- | $C_{30}H_{30}FN_3O_5$ | Aniline, $4-[2',3'-benzo-4'-oxo-5'-(2-methoxy-5-$ |
| CHNO | N,O]- 10.77 | C II O | fluorosulfonylphenyl)amino-N,N'-diphenyl- 9.33 |
| $C_{26}H_{27}N_3O_2$ | Aniline, 4-[N-benzoyl(phenylaminocarbonyl)-methylene]amino-N,N-diethyl-3-methyl- 9.13 | $C_{30}H_{40}O$ | β-8'-Carotenal (apo) 2.125 β-8'-Carotenol (apo) 2.126 |
| $C_{26}H_{32}N_2NiO_2$ | Nickel(II), bis[2-[(cyclohexylimino)methyl]phenolato- | $C_{30}H_{42}O \\ C_{30}H_{42}O_{2}$ | 2,5-Cyclohexadien-4-one, 1,2-ethanediylidenebis[3,5- |
| 026113211211102 | N,O - 10.84 | $C_{30}\Pi_{42}C_{2}$ | di(2-methyl-2-propyl)- 15.20 |
| $C_{26}H_{34}CoO_4$ | Cobalt(II), bis[2-hydroxy-3,5-di(2-propyl)benzoato- | $C_{30}H_{44}$ | Carotene analog, C-30 2.121 |
| | <i>O</i> , <i>O</i> ']- 10.69 | $C_{30}H_{45}NNiO_2S$ | Nickel(II), ethaneamine[2,2'-thiobis-4-(1,1,3,3- |
| $C_{26}H_{34}NiO_4$ | Nickel(II), bis[2-hydroxy-3,5-di(2-propyl)benzoato- | | tetramethylbutyl)phenolato-0,0']- 10.101 |
| 0 H N | 0,0']- 10.70 | $\mathrm{C_{30}H_{48}CoN_2S_4}$ | Cobaltate(II), bis[toluene-3,4-dithiolato(2-)-S,S']-, |
| $C_{27}H_{21}N$ | Anthracene, 1-methylamino-9,10-diphenyl- 3.58 4,5,4',5'-Dibenzo-2,2'-thiacyanine, 3,3'-diethyl-, | C U N N;S | di(tetrabutylammonium) 10.51 Nickelate(II), bis[toluene–3,4–dithiolato(2–)–5,5']–, |
| $C_{27}H_{23}CIN_2S_2$ | chloride 9.35 | $\mathrm{C}_{30}\mathrm{H}_{48}\mathrm{N}_{2}\mathrm{NiS}_{4}$ | di(tetrabutylammonium) 10.52 |
| $C_{27}H_{26}N_2O_3S_3$ | 2,2'-Thiacarbocyanine, 3,3'-diethyl-, toluenesulfonate | $C_{31}H_{29}BrN_2S_2$ | 4,5,4',5'-Dibenzo-2,2'-thiacarbocyanine, 3,9,3'-triethyl- |
| -2720 2-3-3 | 9.37 | 31 29 2 2 | , bromide 9.46 |
| $C_{27}H_{28}N_2O_2$ | Aniline, 4-(dibenzoylmethylene)amino-3,N,N-triethyl- | $C_{31}H_{30}N_2O_3S$ | 4,4'-Carbocyanine, 1,1'-diethyl-, toluenesulfonate 9.41 |
| | 9.8 | $C_{31}H_{32}IN_3$ | 2,2'-Carbocyanine, 1,3,3,1',3',3'-hexamethyl-8,10- |
| $C_{27}H_{29}N_3O_2$ | Aniline, 4-[N-benzoyl(phenylaminocarbonyl)- | | indolo-, iodide 9.48 |
| CHNO | methylene]amino-3,5-dimethyl-N,N-diethyl- 9.14 Aniline, 4-[N-di(phenylaminocarbonyl)methylene]- | $C_{31}H_{34}N_2O_5S_3$ | 2,2'-Thiacarbocyanine, 3,9,3-triethyl-5,5'-dimethoxy-, toluenesulfonate 9.43 |
| $\mathrm{C_{27}H_{30}N_4O_2}$ | amino-3-N,N-triethyl- 9.9 | $C_{31}H_{47}NNiO_2S$ | Nickel(II), propaneamine[2,2'-thiobis-4-(1,1,3,3- |
| $C_{27}H_{46}O$ | Cholesterol 14.9 | 031114/11111020 | tetramethylbutyl)phenolato-O,O']- 10.103 |
| $C_{27}^{27}H_{46}^{46}O_{2}$ | δ-Tocopherol 4.25 | $C_{31}H_{50}O_2$ | Stigmasteryl acetate 14.13 |
| $\mathrm{C_{28}H_{14}O_2}$ | 1,2,7,8-Dibenzperylene-3,9-quinone 3.66 | $C_{31}H_{52}O_2$ | Sitosteryl acetate 14.14 |
| $\mathrm{C_{28}H_{20}N_2O}$ | Aniline, 4-(2',3'-benzo-4'-oxocyclohexa- | $C_{31}H_{52}O_3$ | α-Tocopheryl acetate 14.3 |
| C II N:C2- | dienylidene)amino-N,N-diphenyl- 9.32 | $C_{32}H_{22}O$ | Isobenzofuran, 1,3,4,7-tetraphenyl- 5.38 |
| $C_{28}H_{20}NiS_4^{2-}$ | Nickelate(II) ion, bis(1,2-diphenylethanedithionato(2-)- S,S')- 10.50 | $C_{32}H_{44}O_2$ $C_{32}H_{49}CoNO_2S$ | β-8'-Carotenoic acid, ethyl ester (apo) 2.127 Cobalt(II), butaneamine[2,2'-thiobis-4-(1,1,3,3- |
| $C_{28}H_{20}O$ | Furan, 2,3,4,5-tetraphenyl- 5.33 79A106 | C321149C011O25 | tetramethylbutyl)phenolato- $0,0'$]- 10.104 |
| $C_{28}H_{20}O_2$ | p-Dioxin, tetraphenyl- 79A241 | C ₃₂ H ₄₉ NNiO ₂ S | Nickel(II), butaneamine[2,2'-thiobis-4-(1,1,3,3- |
| $C_{28}H_{22}N_4O$ | 2-Pyrazolin-5-one, 4-(4'-diphenylaminophenyl)imino- | ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | tetramethylbutyl)phenolato-0,0']- 10.105 |
| | 3-methyl-1-phenyl- 9.27 | $C_{33}H_{34}N_4O_6$ | Biliverdine 14.34 |
| $C_{28}H_{22}NiO_4$ | Nickel(II), bis(2-hydroxy-5-methylbenzophenonato- | $C_{33}H_{36}N_4O_6$ | Bilirubin 14.32 79A111 |
| G H 0 | 0,0')- 10.63 | $C_{34}H_{34}NiO_6$ | Nickel(II), bis[2-hydroxy-4-(2-methyl-2-propyl)-phenylbenzoato-0,0']- 10.68 |
| $C_{28}H_{22}O_2$ | Anthracene, 1,4-dimethoxy-9,10-diphenyl- 3.59 Cobalt(II), bis(O,O'-di-4-methylphenyldithio- | C ₃₄ H ₄₅ NNiO ₂ S | Nickel(II), benzeneamine[2,2'-thiobis-4-(1,1,3,3- |
| C ₂₈ H ₂₈ C0O ₄ F ₂ S ₂ | phosphato- S , S')- 10.37 | 034114511111020 | tetramethyl)phenolato-O,O']- 10.109 |
| CooHooCuO4PoS | Copper(II), bis(O,O'-di-4-methylphenyldithio- | $C_{34}H_{50}N_2NiO_2$ | Nickel(II), 2,2'-[1,2-ethanediylbis(nitrilo- |
| 20 20 7 2 | phosphato-S,S')- 10.39 | | decylidene)]bis[4-methylphenolato(2-)- N , N' , O , O']- |
| $C_{28}H_{28}NiO_4P_2S_4$ | Nickel(II), $bis(O, O'-di-4-methylphenyldithio-$ | 0.11.0 | 10.95 |
| | phosphato-S,S')- 10.38 | $C_{34}H_{50}O_2$ | Cholesteryl benzoate 14.10 Nickel(II), cyclohexaneamine[2,2'-thiobis-4-(1,1,3,3- |
| $C_{28}H_{29}N_5O_2$ | 2-Pyrazolin-5-one, 4-(4'-diethylamino-2',6'-dimethylphenyl)-imino-3-(benzoylamino)-1-phenyl- | $C_{34}H_{51}NNiO_2S$ | Nickel(II), cyclohexaneamine[$2,2$ '-thiobis-4-($1,1,3,3$ -tetramethylbutyl)phenolato- $0,0$ ']- 10.107 |
| | 9.26 | · C ₃₄ H ₅₃ NNiO ₅ S | Nickel(II), nitrilotris(2-hydroxyethyl)[2,2'-thiobis-4- |
| $C_{28}H_{40}NiO_2S$ | Nickel(II), bis[2,2'-thiobis-4-(1,1,3,3-tetramethyl- | - 34 -33 30 | (1,1,3,3-tetramethylbutyl)phenolato $-O,O'$]- 10.113 |
| -2040 | butyl)phenolato-0,0']- 10.114 | $\mathrm{C_{34}H_{56}NiO_8P_2}$ | Nickel(II), bis[O-ethyl-[3,5-di-(2-methyl-2-propyl)- |
| $\mathrm{C_{28}H_{41}NNiO_{2}S}$ | Nickel(II), dodecaneamine[2,2'-thiobis(3,4-dimethyl)- | | 4-hydroxybenzyl]phosphonato-0,0']- 10.22 |
| | phenolato-0,0']- 10.111 | $C_{35}H_{30}N_2O_3S_3$ | 4,5,4',5'-Dibenzo-2,2'-thiacarbocyanine, 3,3'-diethyl-, |
| $C_{28}H_{42}NiO_3S$ | Nickel(II), aqua[2,2'-thiobis-4-(1,1,3,3-tetramethyl- | $C_{35}H_{38}N_4O_6$ | toluenesulfonate 9.40 Biliverdine dimethyl ester 14.35 |
| | butyl)phenolato $-0,0$]- 10.98 | U351138114U6 | Difference dimension to contract 17:00 |

| 984 | L' MITVILIZOIA VI | ID J. DROMM | |
|--|---|---|--|
| $C_{35}H_{50}$ | Carotene analog, C-35 2.123 | $Cl_2H_{12}MnO_6$ | Manganese(II |
| $C_{35}H_{62}O_3$ | Benzenepropanoic acid, 4-hydroxy-3,5-di(2-methyl-2- | $Cl_2H_{12}NiO_6$ | Nickel(II) ion |
| | propyl)-, octadecyl ester 4.17 | D_2O | Water-d ₂ 1.2 |
| $C_{36}H_{24}N_{10}N_1$ | Nickel(II), bis[1,3-bis(2-pyridylimino)isoindolinato- | H ₂ O | Water 1.1 1. |
| CHO | N,N',N'']- 10.115 | I- N - | Iodide ion 12 |
| $C_{38}H_{58}O_4$ | 2,5-Cyclohexadien-4-one, 1,2-ethanediylidenebis[3-[2-hydroxy-5-methyl-3-(2-methyl-2-propyl)benzyl]-5- | $N_3^ O_2$ | Azide ion 12. Oxygen $({}^{3}\Sigma_{g})$ |
| | (2-methyl-2-propyl)]- 4.33 | O_2^{-} | Superoxide io |
| C38H60C0N2O2 | Cobalt(II), bis[2-[(dodecylimino)methyl]phenolato-N,O]- | ~ ₂ | ouporomide to |
| 38 00 - 2-2 | 10.88 | | |
| $\mathrm{C_{38}H_{60}CuN_{2}O_{2}}$ | Copper(II), bis[2-[(dodecylimino)methyl]phenolato- | | |
| G W N N | N,O]- 10.90 | | _ |
| $\mathrm{C_{38}H_{60}N_2NiO_2}$ | Nickel(II), bis[2-[(dodecylimino)methyl]phenolato-N,O]- | | Compou |
| C ₃₈ H ₆₄ NiO ₈ P ₂ | 10.89 Nickel(II), bis[O-butyl-[3,5-di-(2-methyl-2-propyl)- | | |
| C ₃₈ H ₆₄ MO ₈ F ₂ | Nickel(II), bis[O-butyl-[3,5-di-(2-methyl-2-propyl)-4-hydroxybenzyl]phosphonato-O,O']- 10.23 | The semne | ound name inde |
| C39H62N2NiO4 | Nickel(II), bis(2-hydroxy-4-methyldodecanophenone | • | me. Each name |
| 39 62 2 - 4 | oximato- N , O)- 10.75 | • | tables 1 thru 1 |
| $C_{40}H_{48}CdO_4P_2S$ | S_4 Cadmium(II), bis[2,2'-thiobis[0,0'-di-4-(2-methyl- | | ntly Published R |
| | 2-propyl)phenyl]dithiophosphato-S,S']- 10.43 | | • |
| $C_{40}H_{48}CoO_4P_2S$ | 64 Cobalt(II), bis[2,2'-thiobis[0,0'-di-4-(2-methyl- | Acetic acid, e | thyl ester 1.28 |
| C H NO D C | 2-propyl)phenyl]dithiophosphato-S,S']- 10.40 | Acetone 1.22 | |
| C ₄₀ H ₄₈ N1O ₄ P ₂ S | Nickel(II), bis[2,2'-thiobis[0,0'-di-4-(2-methyl- | Acetone-d ₆ 1a | |
| СНОРРЫ | 2-propyl)phenyl]dithiophosphato-S,S']- 10.41 Lead(II), bis[2,2'-thiobis[0,0'-di-4-(2-methyl- | Acetone oxime Acetonitrile 1 | |
| O401148O41 21 DC | 2-propyl)phenyl]dithiophosphato-S,S']- 10.44 | Acrolein 2.22 | |
| C40H48O4P2S4Z | | | , adamantylidene- |
| T/ W/ T 2 T | 2-propyl)phenyl]dithiophosphato-S,S']- 10.42 | Adenine 14.3 | • |
| C ₄₀ H ₅₂ CoO ₄ P ₂ S | S ₄ Cobalt(II), bis[O,O'-di-4-(2-methyl-2-propyl)phenyl- | Adenosine 14 | |
| | dithiophosphato-S,S']- 10.34 | Aetiobilirubin | -IV-γ 14.33 |
| $C_{40}H_{52}CuO_4P_2S$ | S_4 Copper(II), bis[O , O' -di- 4 -(2-methyl-2-propyl)phenyl- | Alanine 79A | |
| C H NO D C | dithiophosphato-S,S']- 10.36 | | 3,4-dihydroxyphe |
| C ₄₀ H ₅₂ NiO ₄ P ₂ S | is Nickel(II), bis[0,0'-di-4-(2-methyl-2-propyl)phenyl- | Alloocimine-A | |
| $C_{40}H_{52}O_2$ | dithiophosphato-S,S']- 10.35 Canthaxanthin 2.131 | Anethole 3.2 | hloride, dodecyl R |
| C ₄₀ H ₅₆ | β -Carotene 2.130 79F463 | Aniline 7.1 | 6 |
| 40 30 | Lycopene 2.132 | | ',3'-benzo-4'-ox |
| $C_{40}H_{56}O_2$ | Isozeaxanthin 2.129 | | 9.31 |
| | Lutein 2.128 | Aniline, 4–(2 | ',3'-benzo-4'-ox |
| $C_{40}H_{62}$ | Sarcina phytofluene 2.120 | | diphenyl- 9.3 |
| C ₄₀ H ₆₄ | Sarcina phytoene 2.118 | Aniline, 4-[2 | ',3'-benzo-4'-ox |
| C ₄₀ H ₆₅ NNiO ₂ S | Nickel(II), bisdodecaneamine[2,2'-thiobis(3,4-dimethyl)phenolato-0,0']- 10.112 | Anilina A IA | .–phenyl)amino V–benzoyl(phenyl |
| | Nickel(II), dodecaneamine[2,2'-thiobis-4-(1,1,3,3- | Amme, 4-[/ | diethyl- 9.12 |
| | tetramethylbutyl)phenolato-0,0']- 10.110 | Aniline, 4-IA | /-benzoyl(phenyl |
| $C_{42}H_{28}$ | Naphthacene, 5,6,11,12-tetraphenyl- 3.63 | , . | diethyl-3-metl |
| $\mathrm{C_{42}H_{38}N_4Ni}$ | Nickel(II), bis[1-(4'-methylphenyl)amino-2-(4'- | Aniline, 4-[A | /_benzoyl(phenyl |
| | methylphenyl)iminocycloheptatriene-N,N']- 10.47 | | dimethyl-N,N- |
| C ₄₄ H ₂₈ CoN ₄ ⁺ | Cobalt(III), tetraphenylporphinato- 10.120 | | omo– <i>N,N</i> –dimetl |
| C ₄₄ H ₂₈ CuN ₄ | Copper(II), tetraphenylporphinato- 10.118 | | hloro–N,N–dimet |
| C ₄₄ H ₂₈ N ₄ Ni C ₄₄ H ₂₈ N ₄ Zn | Nickel(II), tetraphenylporphinato- 10.117 Zinc(II), tetraphenylporphinato- 10.119 | | ano– <i>N,N</i> –dimeth libenzoylmethyler |
| $C_{44}H_{28}N_4$ | Porphine, tetraphenyl- 14.30 | | -diethyl-3,5-dim |
| C44H30O | Isobenzofuran, 1,3,4,5,6,7-hexaphenyl- 5.39 | , | hexadienyliden |
| $C_{44}H_{32}N_4Zn$ | Zinc(II), tetraphenylchlorinato- 10.122 | Aniline, N,N | -diethyl-3-meth |
| $C_{44}H_{34}N_4$ | Bacteriochlorin, tetraphenyl- (trans) 14.29 | | methylene]ami |
| $C_{46}H_{31}FeN_4O_2$ | lron(III), (acetato)tetraphenylporphinato- 10.121 | Aniline, N,N | -diethyl-4-[<i>N</i> -(p |
| C ₄₇ H ₃₉ ClO ₆ | Pyrylium, 2,3,2',3'-bis(1,4,10,13-trideca-4,6,8,10- | 4 (1) 37 37 | amino- 9.10 |
| СПО | tetraen)tetrayl[4,6-diphenyl-, perchlorate 9.54 | | -dimethyl- 7.6 |
| $C_{50}H_{72}O_2 \\ C_{50}H_{74}O_2$ | P-438 2.124 P-422 2.122 | Annine, 4-[/ | V-di(phenylamino 9.15 |
| C ₅₅ H ₇₀ MgN ₄ O ₅ | | Aniline, 4-1/ | V–di(phenylamino |
| $C_{55}H_{70}N_4O_5$ | Protopheophytin 14.27 | , *-[1 | 9.9 |
| $C_{55}H_{72}MgN_4O$ | | Aniline, 4-(/ | V-dipivaloylmeth |
| $C_{55}H_{72}N_4O_5$ | Pheophytin a 14.26 | | nethoxy <i>–N,N–</i> din |
| C ₅₅ H ₇₄ MgN ₄ O | • • | Aniline, p-m | ethoxy- <i>N,N</i> -dim |
| $C_{55}H_{74}N_4O_6$ | Bacteriopheophytin a 14.28 | Aniline, N-n | |
| $C_{56}H_{96}N_2O_4Pd$ | | • | ethyl-N,N-dime |
| Q1 ₀ | octadecanophenone oximato-N,O]- 10.74 | Anisole 3.4 | dia Luari 4 |
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| Cl ₂ CoH ₁₂ O ₆ | Cobalt(II) ion, hexaaqua-, dichloride 10.2 | | 3-methyl–2-bute 3-methvl–2-bute |

| Cl ₂ H ₁₂ MnO ₆ | Manganese(II) ion, hexaaqua-, dichloride 10.3 |
|--|---|
| Cl ₂ H ₁₂ NiO ₆ | Nickel(II) ion, hexaaqua-, dichloride 10.1 |
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| H_2O | Water 1.1 1.38 1.48 79N041 |
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Cl₂H₈MnO₄

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Carotene analog, C-30 2.121
                                                                             Cyclohexane, 1,4-dichloro-1,4-dinitroso- (trans) 13.8
Carotene analog, C-35 2.123
                                                                              Cyclohexane, ethylidene- 2.8
β-Carotene 2.130 79F463
                                                                             Cyclohexane, methylidene- 2.7
β-8'-Carotenoic acid, ethyl ester (apo) 2.127
                                                                             Cyclohexanol 1.31
β-8'-Carotenol (apo) 2.126
                                                                              Cyclohexanol, 2-cyclohexylidene- 2.14
Carvomethene 2.60
                                                                             Cyclohexanone, 2-cyclohexylidene- 2.15
Caryophyllene (-) 2.111
                                                                             Cyclohexene 2.54
Chloride ion 12.1
                                                                              Cyclohexene, 1,2-dimethyl- 2.58
Chloroform 1.5 79E699
                                                                             Cyclohexene, 2,3-dimethyl- 2.59
Chloroform-d 1.6
                                                                             Cyclohexene, 3,6-endoperoxy- 2.62
Chlorophyll a 14.23
                                                                              Cyclohexene, 1-methyl- 2.56
Chloropromazine 11.38
                                                                             Cyclohexene, 4-methyl- 2.57
Cholesterol 14.9
                                                                             Cyclohexylamine 6.7
Cholesteryl benzoate 14.10
                                                                              Cyclooctatetraene dibromide 2.117
 \hbox{6--Chromanol, 2,8--dimethyl-2-(4,8,12-trimethyltridecyl)-} \quad \textbf{4.25} \\
                                                                             Cyclooctene 2.83
6-Chromanol, 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)- 4.28
                                                                             Cyclooctene, 1-methyl- 2.84
6-Chromanol, 2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-, acetate
                                                                              Cyclopentadiene 2.86 79A106
                                                                              4H-Cyclopentadieno[b]quinoline, 1,2-diphenyl-4-methyl- 5.46
               14.3
                                                                              Cyclopentadienone, tetraphenyl- 3.38
6-Chromanol, 2,5,8-trimethyl-2-(4,8,12-trimethyltridecyl)- 4.26
6-Chromanol, 2,7,8-trimethyl-2-(4,8,12-trimethyltridecyl)- 4.27
                                                                              Cyclopentane, (dicyclopropylmethylidene)- 2.20
Chromium(II), bis(O,O'-diphenyldithiophosphato-S,S')- 10.32
                                                                              Cyclopentane, ethylidene- 2.6
Chromium(III), tris(2,4-pentanedionato-0,0')- 10.58
                                                                              Cyclopentane, methylidene- 2.5
β-Citronellol 2.82
                                                                              Cyclopentene 2.50
Cobalt(II), bis(N,N-dibutyldithiocarbamato-S,S')- 10.16
                                                                              Cyclopentene, 1-methyl- 2.52
Cobalt(II), bis(O,O'-dicyclohexyldithiophosphato-S,S')- 10.26
                                                                              Cyclopropane, (dicyclopropylmethylidene)- 79F119
Cobalt(II), bis(O,O'-di-4-methylphenyldithiophosphato-S,S')- 10.37
                                                                              Cyclopropane, (dicyclopropylmethylidene)- 2.18
                                                                              Cyclopropane, (dimethylmethylidene)- 79F119
Cobalt(II), bis[O,O'-di-4-(2-methyl-2-propyl)phenyldithiophosphato-
                                                                              Cytidine 14.40
               S,S'|- 10.34
                                                                              DABCO 6.40
Cobalt(II), bis(O,O'-diphenyldithiophosphato-S,S')- 10.28
                                                                              1,6-Decadiene, 2,6,9-trimethyl- (cis) 2.108
Cobalt(II), bis(N,N-di-2-propyldithiocarbamato-S,S')- 10.11
                                                                              1,6-Decadiene, 2,6,9-trimethyl- (trans) 2.107
Cobalt(II), bis[2-[(dodecylimino)methyl]phenolato-N,O]- 10.88
                                                                              7-Dehydroandrosterone-3-acetate 14.16
Cobalt(II), bis[2-hydroxy-3,5-di(2-propyl)benzoato-0,0']- 10.69
                                                                              16-Dehydropregnenolone-3-acetate 14.15
Cobalt(II), bis(2,4-pentanedionato-0,0')- 10.54
                                                                              1,4-Diazabicyclo[2.2.2]octane 6.40 79F463
Cobalt(II), bis[2-[(phenylimino)methyl]phenolato-N,O]- 10.85
                                                                              2,3-Diazabicyclo[2.2.2]oct-2-ene-2,3-dioxide, 1,4-dichloro- 13.10
Cobalt(II), bis[2,2'-thiobis[0,0'-di-4-(2-methyl-2-propyl)phenyl]-
                                                                              1,4-Diazacyclohexane 6.39
               dithiophosphato-S,S']- 10.40
                                                                              2,3-Diazahexacyclo[5.4.2.0.1.110.4.1206.10]tridec-2-ene-2,3-dioxide, 1,4-
Cobalt(II), butaneamine[2,2'-thiobis-4-(1,1,3,3-tetramethylbutyl)-
               phenolato-0,0']- 10.104
                                                                                            dichloro- 13.11
                                                                              9.Diazofluorene 9.6
Cobalt(II), 2,2'-[1,2-ethanediylbis(nitrilomethylidyne)]bis[phenolato-(2-)-
                                                                              Diazomethane, (4-bromophenyl)phenyl 9.2
               N,N′,O,O′]- 10.92
Cobalt(II) ion, hexaaqua-, dichloride 10.2
                                                                              Diazomethane, di(4-chlorophenyl) 9.4
                                                                              Diazomethane, di(4-methylphenyl) 9.5
 Cobalt(III), tetraphenylporphinato- 10.120
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Diazomethane, diphenyl 9.1

Cobalt(III), tris(2,4-pentanedionato-0,0')- 10.61

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Diazomethane, (4-methoxyphenyl)phenyl 9.3
 1,2,5,6-Dibenzanthracene 3.64
 4,5,4',5'-Dibenzo-2,2'-thiacarbocyanine, 3,3'-diethyl-, toluenesulfonate
                9.40
 4,5,4',5'-Dibenzo-2,2'-thiacarbocyanine, 3,9,3'-triethyl-, bromide 9.46
 4,5,4',5'-Dibenzo-2,2'-thiacyanine, 3,3'-diethyl-, chloride 9.35
 1,2,7,8-Dibenzperylene-3,9-quinone 3.66
 Diethylamine 6.12
 Diethylamine, N-(7-aminoheptyl)- 6.27
 Diethylamine, N-(2-cyanoethyl)- 6.26
 Diethylamine, N-(2-hydroxyethyl)- 6.24
 Diethylamine, 2-methoxyethyl- 6.25
 Diisopropylamine 6.14
 7,8-Dioxabicyclo[2.2.2]oct-2-ene 2.62
 1,4-Dioxacyclohexadiene, tetraphenyl- 79A241
 3.6-Dioxacyclohexene 2.55
 3,6-Dioxacyclohexene, 1,2-diphenyl- 2.63
                                                                             Ethylamine 6.1
 3,5-Dioxacyclopentene 2.51
 Dioxane 1.27 15.19
 13,14-Dioxatricyclo[8.2.1.1<sup>4,7</sup>]tetradeca-4,6,10,12-tetraene 5.34
                                                                             Ferrocene 10.123
 p-Dioxene, 2,3-diphenyl- 2.63
 p-Dioxene 2.55
 p-Dioxin, tetraphenyl- 79A241
                                                                             Freon 11 1.7
 1,3-Dioxole 2.51
                                                                             Freon-113 1a.2
 Diphenylamine 7.4
 Diphenylamine, 4,4'-di(1,1,3,3-tetramethylbutyl)- 7.5
 Dipropylamine 6.13
 Dipyrromethane, 4,4'-diethyl-3,5,3',5'-tetramethyl-(2.2')- 79F118
 Dipyrromethene, 4,4'-diethyl-3,5,3',5'-tetramethyl-(2.2')- 79F118
 [2.2']-Dipyrromethene, 5'-oxo-3',4'-diethyl-5-methyl-1',5'-dihydro-
               14.21
[2.2']-Dipyrromethene, 5'-oxo-4-ethyl-3,5-dimethyl-1',5'-dihydro-
               14.22 79A113
Dipyrromethene, 5'-oxo-3'-ethyl-4',5'-dimethyl-1',5'-dihydro-(2.2')-
               79A113
Dipyrromethene, 5'-oxo-4-ethyl-3,5-dimethyl-1',5'-dihydro-(2.2')-
               79A113
[2.2']-Dipyrromethene, 5'-oxo-3'-ethyl-4',3,5-trimethyl-1',5'-dihydro-
               14.19
[2.2']-Dipyrromethene, 5'-oxo-3',4',4-triethyl-3,5-dimethyl-1',5'-
              dihydro- 14.18 79A113
[2.2']-Dipyrromethene, 5'-oxo-4',4,5-trimethyl-3'-ethyl-1',5'-dihydro-
               14.20
[2.2']-Dipyrromethene, 5'-oxo-4'-vinyl-4-ethyl-3',3,5-trimethyl-1',5'-
               dihydro- 14.17 79A113
Disulfide, diethyl 11.39
1,4-Dithiane 11.40
Dithiocarbamate ion, dimethyl- 11.41
Dithiocarbamate ion, hexamethylene- 11.42
5-[3-(1,2-Dithiolanyl)]pentanoic acid 11.45
1,3-Dithiole-2-thione, 4,5-diphenyl- 11.46
4,8-Dodecadiene, 4,8-dimethyl-(trans,trans)- 2.112
4,8-Dodecadiene, 4,8-dimethyl- 2.113
4,8-Dodecadiene, 4,8-dimethyl-, mixture of hydroperoxides obtained
                                                                            Furan, 2-vinyl- 5.9
              from its photosensitized oxygenation. 2.114
Dopa 79F315
Dregamine 6.31
Durohydroquinone monoethyl ether 4.24
Ergosterol 14.11
Ethane, 1,1-dichloro- 1.13
Ethane, 1,2-dihydroxy- 1.11 1.40
Ethane, dithiobis- 11.39
Ethane, iodo- 15.4
Ethane, 1,1,2,2-tetrachloro- 1.18
Ethane, thiobis- 11.14
Ethane, 1,2,2-trichloro-1,1,2-trifluoro- 1a.2
Ethanol 1.10 1.48 15.3 79E699
Ethanol, 2-butoxy- la.4
Ethanol, 2-cyclododecylidene- 79F137
Ethanol, 2-cyclohexylidene- 79F137
                                                                            Furfural 5.4
Ethanol, 2-cyclooctylidene- 79F137
                                                                            Furfuryl alcohol 5.6
Ethanol, 2-cyclopentylidene- 79F137
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Ethanol, 2,2-dichloro- 1.14
 Ethanol, 2-(N,N-diethylamino)- 6.24
 Ethanol, 2-fluoro- 1.12
 Ethanol, 2,2'-thiobis- 11.16
 Ethanol, 2,2,2-trichloro- 1.15
 Ethanol, 2,2,2-trifluoro- 1.16
 Ethene, 1,2-diethoxy- (cis) 2.3
 Ethene, 1,2-diethoxy- (trans) 2.4
 Ethene, 1,1-diethoxy- 2.2
 Ethene, ethoxy- 2.1
 Ethene, 1,1,2,2-tetraethoxy- 2.12
 Ethene, 1,1,2-tricyclopropyl- 2.10
 Ethene, 1,1,2-triethoxy- 2.9
 Ether, ethyl vinyl 2.1
 Ether, furfuryl methyl 5.7
 Ethyl ether 79E699
 Ethylamine, 2-phenyl- 6.9
 Ethylene glycol 1.11 1.40
 Fluoren-9-yl anion, 9-benzenesulfonyl 11.47
 Formamide, N,N-dimethyl- 1.21 6.20
 Fulvene, 6,6-dimethyl- 2.115
 Fulvene endoperoxide, 6,6-dimethyl- 2.87
 Furan 5.1 79A106
 Furan, 2-acetyl- 5.17
 Furan, 3-(4'-bromophenyl)- 5.23
 Furan, 2-(4'-chlorophenyl)- 5.22
 Furan, 2,5-di(4-chlorophenyl)- 79A106
 Furan, 3,4-diethoxycarbonyl- 5.32
 Furan, 2,4-dimethyl- 5.28
 Furan, 2,5-dimethyl- 5.29 79A106
 Furan, 2,5-di(2-methyl-2-propyl)- 79A106
 Furan, 2,3-diphenyl- 79A106
 Furan, 2,5-diphenyl- 5.30 79A106
 Furan, 3,4-diphenyl- 5.31
 Furan, 2-ethenyl- 5.9
 Furan, 3-(4'-fluorophenyl)- 5.21
 Furan, 2-(1-hydroxyethyl)- 5.10
Furan, 2-methoxy- 5.5
Furan, 2-(methoxymethyl)- 5.7
Furan, 2-(4'-methoxyphenyl)- 5.26
Furan, 3-(4'-methoxyphenyl)- 5.27
Furan, 2-methyl- 5.2
Furan, 2-(4'-methylphenyl)- 5.24
Furan, 3-(4'-methylphenyl)- 5.25
Furan, 2-phenyl- 5.19
Furan, 3-phenyl- 5.20
Furan, tetrahydro- 1.26 15.11
Furan, 2,3,4,5-tetraphenyl- 5.33 79A106
Furan, 2-(p-\text{tolyl})-5.24
Furan, 3-(p-tolyl)- 5.25
2-Furancarboxaldehyde 5.4
2-Furancarboxylic acid 5.8
3,4-Furandicarboxylic acid, diethyl ester 5.32
2-Furanmethanamine 5.3
2-Furanmethanamine, N-methyl- 5.18
2-Furanmethanol 5.6
2-Furanmethanol, a-benzyl- 5.12
2-Furanmethanol, a,a-diphenyl- 5.16
2-Furanmethanol, \alpha-(diphenylmethyl)- 5.15
2-Furanmethanol, α-methyl- 5.10
2-Furanmethanol, \alpha-(3-phenylpropyl)- 5.14
2-Furanmethanol, α-phenyl- 5.11
2-Furanmethanol, \alpha-(2-phenylethyl)- 5.13
[2.2](2,5)Furanophane 5.34
Furfuryl alcohol, \alpha-benzhydryl- 5.15
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Furfuryl alcohol, α-benzyl- 5.12
                                                                           Methane, thiobis(phenyl)- 11.24
                                                                           Methanol 1.3 1.38 1.39 1.40 1.41 1.42 1.43 1.44 1.45 1.46 1.47
Furfuryl alcohol, a,a-diphenyl- 5.16
                                                                                          1.49 1.50 15.2 1a.10 1a.11 1a.9
Furfuryl alcohol, α-methyl- 5.10
Furfuryl alcohol, a-phenethyl- 5.13
                                                                           Methanol-d<sub>4</sub> 1a.8
                                                                           Methionine 79A112 8.2
Furfuryl alcohol, a-phenyl- 5.11
                                                                           1.-Methionine, CBZ-, methyl ester 8.3
Furfuryl alcohol, \alpha-(3-phenylpropyl)- 5.14
Furfurvlamine 5.3
                                                                           Methylamine, N,N-di(2-hydroxyethyl)- 6.19
                                                                           Methylene chloride 1.4 1a.10 1a.11 1a.9
Furfurylamine, N-methyl- 5.18
2-Furoic acid 5.8
                                                                            Naphthacene 3.62
                                                                            Naphthacene, 5,6,11,12-tetraphenyl- 3.63
Guanosine 14.36
                                                                            1,4-Naphthalendione, 2-methyl- 3.42
Heptane 15.8
Heptane, 3-methyl- 15.9
                                                                            Naphthalene, 2-amino- 7.2
Heptane, 4-methyl- 15.10
                                                                            Naphthalene, 1,4-dimethyl- 3.41
1-Heptene 2.76
                                                                            Naphthalene, 1,2,3,4,5,6,7,8-octahydro- 2.16
Hexadecane 1a.7
                                                                            α-Naphthol 4.29
2,4-Hexadiene (trans, trans) 2.89
                                                                            β-Naphthol 4.30
1,5-Hexadiene 2.88
                                                                            2-Naphthylamine 7.2
2,4-Hexadiene, 2,5-dimethyl- 2.90
                                                                            Negopex B 10.75
Hexamethylenetetramine 6.41
                                                                            Nickel (II), \ ammine [2,2'-thiobis-4-(1,1,3,3-tetramethylbutyl) phenolato-\\
2-Hexene 2.53
                                                                                          0,0']- 10.100
Histamine 5.50
                                                                            Nickel(II), aqua[2,2'-thiobis-(3,4-dimethyl)phenolato-0,0']- 10.99
Histidine 79A112 8.7
                                                                            Nickel(II), aqua[2,2'-thiobis-4-(1,1,3,3-tetramethylbutyl)phenolato-
Hydroquinone 4.31
                                                                                          0.0[- 10.98
Imidazole 5.49
                                                                            Nickel(II), benzeneamine[2,2'-thiobis-4-(1,1,3,3-tetramethyl)phenolato-
Imidazole, 4-(2'-aminoethyl)- 5.50
                                                                                          0,0']- 10.109
Indene 3.40
                                                                            Nickel(II), (3,11-bisacetyl-4,10-dimethyl-1,5,9,13-tetraazacyclo-
Indole 79A106
                                                                                          pentadeca-1,3,9,11-tetraene-N,N',N'',N''')- 10.116
Indole, 2,3-dimethyl- 79A106
                                                                            Nickel(II), bis[2-[(4-aminophenylimino)methyl]phenolato-N,O]- 10.91
Indole, 3-methyl- 79A106
                                                                            Nickel(II), bis[1,3-bis(2-pyridylimino)isoindolinato-N,N',N'']- 10.115
Indole, 3-methyl-2-phenyl- 79A106
                                                                            Nickel(II), bis[4-bromo-2-[(butylimino)methyl]phenolato-N,O]- 10.80
                                                                            Iodide ion 12.5 12.6 12.7 12.8
Iron(II), bis(cyclopentadienyl)- 10.123
                                                                                          phosphonato-O,O']- 10.23
Iron(III), (acetato)tetraphenylporphinato- 10.121
                                                                            Nickel(II), bis[2-[(butylimino)methyl]-4-methoxyphenolato-N,O]- 10.81
Iron(III), tris(N,N-di-2-propyldithiocarbamato-S,S')- 10.15
                                                                            Nickel(II), bis[2-[(butylimino)methyl]phenolato-N,O]- 10.79
Iron(III), tris(2,4-pentanedionato-0,0')- 10.60
                                                                            Nickel(II), bis[2-[(cyclohexylimino)methyl]phenolato-N,O]- 10.84
Isobenzofuran 5.35
                                                                            Nickel(II), bis(N,N-\text{dibutyldithiocarbamato}-S,S')- 10.17
 Isobenzofuran, 5,6-dimethyl-1,3-diphenyl- 5.37
                                                                            Nickel(II), bis(dicyclohexyldithiophosphinato-S,S')- 10.27
 Isobenzofuran, 1,3-diphenyl- 5.36 79A106
                                                 79E106 79E611
                                                                            Nickel(II), bis(N,N-diethyldithiocarbamato-S,S')- 10.9
               79F643 79N020 79N041
                                                                            Nickel(II), bis(0,0'-diethyldithiophosphato-S,S')- 10.24
 Isobenzofuran, 1,3,4,5,6,7-hexaphenyl- 5.39
                                                                            Nickel(II), bis(N,N-dimethyldithiocarbamato-S,S')- 10.8
 Isobenzofuran, 1,3,4,7-tetraphenyl- 5.38
                                                                            Nickel(II), bis(O, O'-di-4-methylphenyldithiophosphato-S, S')- 10.38
 Isobutenylamine, N,N-dimethyl- 6.21
                                                                            Nickel (II), \ bis [\textit{O}, \textit{O'}-di-4-(2-methyl-2-propyl) phenyl dithiophosphato-
 Isobutylamine 6.5
                                                                                          S,S']- 10.35
 Isobutylene 2.21
                                                                            Nickel(II), bis(N,N-diphenyldithiocarbamato-S,S')- 10.20
 Isopropylamine 6.3
                                                                            Nickel(II), bis(O,O'-diphenyldithiophosphato-S,S')- 10.29
 Isozeaxanthin 2.129
                                                                            Nickel(II), bis(N,N-di-2-propyldithiocarbamato-S,S')- 10.12
 Kryptocyanine 9.41
                                                                            Nickel(II), bis(O,O'-di-2-propyldithiophosphato-S,S')- 10.25
 Lead(II), bis(O,O'-diphenyldithiophosphato-S,S')- 10.33
                                                                            Nickel(II), bisdodecaneamine[2,2'-thiobis(3,4-dimethyl)phenolato-0,0']-
 Lead(II), bis[2,2'-thiobis[0,0'-di-4-(2-methyl-2-propyl)phenyl]-
                                                                                          10.112
               dithiophosphato-S,S']- 10.44
                                                                            Nickel(II), bis[2-[(dodecylimino)methyl]phenolato-N,O]- 10.89
 Leucomalachite green 79F148
                                                                            Nickel(II), bis[O-ethyl-[3,5-di-(2-methyl-2-propyl)-4-hydroxybenzyl]-
 Limonene 2.97
                                                                                          phosphonato-O,O']- 10.22
 Linoleic acid, methyl ester 14.6
                                                                            Nickel(II), bis[hydrotris(1-pyrazolato)borato]- 10.5
                                                                            Nickel(II), bis(2-hydroxyacetophenone oximato-N,O)- 10.72
 Linolenic acid, methyl ester 14.7
 Lipoic acid 11.45
                                                                            Nickel(II), bis(2-hydroxybenzaldehyde oximato-N,O)- 10.71
 Luminol 7.20
                                                                            Nickel(II), bis[2-hydroxy-3,5-di(2-propyl)benzoato-0,0']- 10.70
 Lutein 2.128
                                                                            Nickel(II), bis(2-hydroxy-4-methylacetophenone oximato-N,O)- 10.73
 Lycopene 2.132
                                                                            Nickel(II), bis(2-hydroxy-5-methylbenzophenonato-0,0')- 10.63
 Lysozyme 8.12
                                                                            Nickel(II), bis(2-hydroxy-4-methyldodecanophenone oximato-N,O)-
 Malachite green 79F148
                                                                                           10.75
 Manganese(II), bis(N,N-di-2-propyldithiocarbamato-S,S')- 10.10
                                                                            Nickel(II), bis[2-hydroxy-4-(2-methyl-2-propyl)phenylbenzoato-0,0']-
 Manganese(II) ion, hexaaqua-, dichloride 10.3
                                                                                           10.68
 Manganese(II) ion, tetraaqua-, dichloride 10.4
                                                                            Nickel(II), bis[2-iminomethylphenolato-N,O]- 10.76
 Manganese(III), tris(2,4-pentanedionato-0,0')- 10.59
                                                                            Nickel(II), bis(4-imino-2-pentanonato-N,O)- 10.53
 Menadione 3.42
                                                                            Nickel(II), bis(1-methylamino-2-methyliminocycloheptatriene-N,N')-
 p-Mentha-1,3-diene 2.92
                                                                                           10.46
 p-Mentha-1,5-diene 2.93
                                                                            Nickel(II), bis[1-(4'-methylphenyl)amino-2-(4'-methylphenyl)imino-
 p-Mentha-1,8-diene 2.97
                                                                                           cycloheptatriene-N,N']- 10.47
 p-Menth-1-ene 2.60
                                                                            Nickel(II), bis[N-(p-methylphenyl)]dithiocarbamato-S,S']- 10.21
 Mesoporphyrin-IX, dimethyl ester 14.31
                                                                            Nickel(II), bis[2-[(1-methylpropylimino)methyl]phenolato-N,O]- 10.82
 Methane, chlorotrifluoro- 1.7
                                                                            Nickel(II), bis[2-[(2-methyl-2-propylimino)methyl]-phenolato-N,O]-
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Methane, dichloro- 1.4 1a.10 1a.11 1a.9

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Nickel(II), bis(2,4-pentanedionato-0,0')- 10.55
                                                                             2,6-Octadiene, 2,6-dimethyl- (trans) 2.103
Nickel(II), bis(2,4-pentanedithionato-S,S')- 10.64
                                                                             2,6-Octadiene, 2,7-dimethyl- 2.105
Nickel(II), bis[2-(phenylaminoimino)methyl]phenolato-N,O]- 10.77
                                                                             2,6-Octadiene, 2,6-dimethyl-, mixture of hydroperoxides obtained from
Nickel(II), bis(N-phenyldithiocarbamato-S,S')- 10.7
                                                                                           its photosensitized oxygenation. 2.104
Nickel(II), bis[2-[(phenylimino)methyl]phenolato-N,O]- 10.86
                                                                             2,5-Octadiene, 7-hydroperoxy-2,7-dimethyl- 2.100
Nickel(II), bis(2-propylcarbonothioyl-S,S')- 10.6
                                                                             2,7-Octadiene, 6-hydroperoxy-2,7-dimethyl- 2.106
Nickel(II), bis[2-[(2-propylimino)methyl]phenolato-N,O]- 10.78
                                                                             1,6-Octadiene-2-ol, 3,7-dimethyl- 2.101
Nickel(II), bis(salicylaldehyde oxime) 10.71
                                                                             2,7-Octadien-1-ol, 3,7-dimethyl- 79F137
Nickel(II) bis(salicylaldehyde phenylhydrazone) 10.77
                                                                             Δ9,10-Octalin 2.16
Nickel(II), bis[2,2'-thiobis[0,0'-di-4-(2-methyl-2-propyl)phenyl]-
                                                                             i-Octane 1a.6
              dithiophosphato-S,S']- 10.41
                                                                             2,4,6-Octatriene, 2,6-dimethyl- 2.116
Nickel(II), bis[2,2'-thiobis-4-(1,1,3,3-tetramethylbutyl)phenolato-0,0']-
                                                                             4-Octene, 4-methyl- (cis) 2.79
              10.114
                                                                             4-Octene, 4-methyl- (trans) 2.78
Nickel(II), butaneamine[2,2'-thiobis(3,4-dimethyl)phenolato-0,0']-
                                                                             4-Octene, 4-methyl- 2.80 2.81
              10.106
                                                                             2-Octen-1-ol, 3,4-dimethyl- 79F137
Nickel(II), butaneamine[2,2'-thiobis-4-(1,1,3,3-tetramethylbutyl)-
                                                                             6-Octen-1-ol, 3,7-dimethyl- 2.82
              phenolato-0,0']- 10.105
                                                                             Oleic acid, methyl ester 14.5
Nickel(II), cyclohexaneamine[2,2'-thiobis(3,4-dimethyl)phenolato-O,O']-
                                                                             1-Oxa-4-thiacyclohexane 11.27
               10.108
                                                                             1,4-Oxathiane 11.27
Nickel(II), cyclohexaneamine[2,2'-thiobis-4-(1,1,3,3-tetramethylbutyl)-
                                                                             Oxazole, 2,5-diphenyl- 5.51
              phenolato-O,O']- 10.107
                                                                             Oxygen ({}^{3}\Sigma_{g}) 15.1 79A113
Nickel(II), diaquabis(5-bromo-2-hydroxybenzaldehydato-0,0')- 10.66
                                                                             P-422 2.122
Nickel(II), diaquabis(2-hydroxybenzaldehydato-0,0')- 10.65
                                                                             P-438 2.124
Nickel(II), diaquabis(2-hydroxy-5-methoxybenzaldehydato-0,0')-
                                                                             Phosphite, tributyl- 15.25
               10.67
                                                                             Palladium(II), bis[2-hydroxy-4-(2-methyl-2-propyl)octadecanophenone
Nickel(II), diaquabis(2,4-pentanedionato-0,0')- 10.62
                                                                                           oximato-N,O]- 10.74
Nickel(II), dodecaneamine[2,2'-thiobis(3,4-dimethyl)phenolato-0,0']-
                                                                             Pentacene 3.65
              10.111
                                                                             Pentane, 2,2,4-trimethyl- 1a.6
Nickel(II), dodecaneamine[2,2'-thiobis-4-(1,1,3,3-tetramethylbutyl)-
                                                                             2-Pentene (cis) 2.38
              phenolato-O,O']- 10.110
                                                                             2-Pentene (trans) 2.39
Nickel(II), ethaneamine[2,2'-thiobis(3,4-dimethyl)phenolato-0,0']-
                                                                             1-Pentene 2.37
              10.102
                                                                             2-Pentene, 2,4-dimethyl- 2.47
Nickel(II), ethaneamine[2,2'-thiobis-4-(1,1,3,3-tetramethylbutyl)-
                                                                             2-Pentene, 3-methyl- (cis) 2.42
              phenolato-0,0']- 10.101
                                                                             2-Pentene, 3-methyl- (trans) 2.43
Nickel(II), 2,2'-[1,2-ethanediylbis(nitrilodecylidene)]bis[4-methyl-
                                                                             2-Pentene, 4-methyl- (cis) 2.45
              phenolato(2-)-N,N',O,O']- 10.95
                                                                             2-Pentene, 4-methyl- (trans) 2.46
Nickel(II), 2,2'-[1,2-ethanediylbis(nitriloethylidyne)]bis[phenolato-(2-)-
                                                                             2-Pentene, 2-methyl- 2.40
              N,N',O,O']- 10.94
                                                                             2-Pentene, 2-methyl-4d- 79F155
Nickel(II), 2,2'-[1,2-ethanediylbis(nitrilomethylidyne)]bis[phenolato-(2-)-
                                                                             2-Pentene, 3-methyl- 2.44
              N,N',O,O']- 10.93
                                                                             2-Pentene, 2,3,4-trimethyl- 2.48
Nickel(II) ion, hexaaqua-, dichloride 10.1
                                                                             2-Pentene, 2,4,4-trimethyl- 2.49
Nickel(II), 2,2-[1,8-naphthalenediylbis(nitrilomethylidyne)]bis-
                                                                             2-Pentene-4-ol, 2-methyl- 2.41
              [phenolato(2-)-N,N',O,O']- 10.97
                                                                             2-Penten-1-ol, 3,4-dimethyl- 79F137
Nickel(II), nitrilotris(2-hydroxyethyl)[2,2'-thiobis-4-(1,1,3,3-tetra-
                                                                            2-Penten-1-ol, 3-ethyl- 79F137
              methylbutyl)phenolato-0,0']- 10.113
                                                                             2-Penten-1-ol, 3-methyl- 79F137
Nickel(II), 2,2'-[1,2-phenylenebis(nitrilomethylidyne)]bis[phenolato-(2-)-
                                                                            2-Penten-1-ol, 3,4,4-trimethyl- 79F137
              N,N',O,O']- 10.96
                                                                            Permanax 45 5.48
Nickel(II), propaneamine[2,2'-thiobis-4-(1,1,3,3-tetramethylbutyl)-
                                                                             α-Phellandrene 2.93
              phenolato-0,0']- 10.103
                                                                            Phenol, 4-acetyl-2,6-di(2-methyl-2-propyl)-, 4.10
Nickel(II), tetraphenylporphinato- 10.117
                                                                            Phenol, 4-benzyl-2,6-di(2-methyl-2-propyl)- 4.15
Nickelate(II), bis[toluene-3,4-dithiolato(2-)-S,S']-
                                                                            Phenol, 4-bromo-2,6-di(2-methyl-2-propyl)- 4.5
              , di(tetrabutylammonium) 10.52
                                                                            Phenol, 4-chloro-2,6-di(2-methyl-2-propyl)- 4.6
Nickelate(II) ion, bis(2,3-butanedithionato(2-)-S,S')- 10.48
                                                                            Phenol, 2,6-di(2-methyl-2-propyl)- 4.1
Nickelate(II) ion, bis(1,2-diphenylethanedithionato(2-)-S,S')- 10.50
                                                                            Phenol, 2,6-di(2-methyl-2-propyl)-4-phenyl- 4.14
Nickelate(II) ion, bis(hexafluoro-2,3-butanedithionato(2-)-S,S')- 10.49
                                                                            Phenol, 4-ethoxy-2,3,5,6-tetramethyl- 4.24
Nicotine 6.30
                                                                            Phenol, 4-hydroxymethyl-3,5-di(2-methyl-2-butyl)- 4.9
1-Nonene 2.85
                                                                            Phenol, 4-(1-imidazolyl)- 79F268
Nopadiene 2.98
                                                                            Phenol, 3-methoxy-4,6-di(2-methyl-2-propyl)- 4.16
Nopinene 2.75
                                                                            Phenol, 4-methoxy-2,6-di(2-methyl-2-propyl)- 4.8
Norborna-2,5-diene, 7,7-dimethyl-2-(trimethylsiloxy)- 2.96
                                                                            Phenol, 4-methyl-2,6-di(2-methyl-2-propyl)- 4.7
Norborna-2,5-diene, 2-methyl- 2.94a
                                                                            Phenol, \ 4-(2-methyl-2-propoxy)-2, \\ 6-di(2-methyl-2-propyl)- \ \textbf{4.13}
Norborna-2,5-diene, 2-(trimethylsiloxy)- 2.95
                                                                            Phenol, 2,2'-thiobis[4-(1,1,3,3-tetramethylbutyl)- 4.32
Norbornane, 7,7-dimethyl-2-methylidene- 2.75a
                                                                            Phenol, 2,4,6-tri(2-methyl-2-propyl)- 4.12
Norbornane-3-d, endo-2-methylidene- 2.73
                                                                            Phenol, 2,4,6-triphenyl- 4.22
Norbornane, 2-methylidene- 2.71
                                                                            Phenothiazine 11.36
Norbornane-3-d, exo-2-methylidene- 2.72
                                                                            Phenothiazine, 2-chloro-10-(3-dimethylaminopropyl)- 11.38
Norborn-2-ene, 7,7-dimethyl-2-(trimethylsiloxy)- 2.67
                                                                            Phenothiazine, 10-methyl- 11.37
Norborn-2-ene, 2-methyl- 2.64
                                                                            Phenoxazine 5.52
Norborn-5-ene, 2-methylidene- 2.94b
                                                                            o-Phenylenediamine 7.14
Norborn-2-ene, 2,7,7-trimethyl- 2.66
                                                                            p-Phenylenediamine, N-cyclohexyl-N'-phenyl-, hydrochloride 7.18
Norborn-2-ene, 2-(trimethylsiloxy)- 2.65
                                                                            p-Phenylenediamine, N-cyclohexyl-N'-phenyl- 7.17
2,6-Octadiene, 2,6-dimethyl- (cis) 2.102
                                                                            p-Phenylenediamine, N-phenyl-N'-(2-propyl)- 7.16
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2-Pyrazolin-5-one, 4-(4'-diethylamino-2'-methylphenyl)imino-3-(2-
p-Phenylenediamine, N,N,N',N'-tetramethyl- 7.19
                                                                                                                              methyl-2-propyl)-1-phenyl- 9.24
Pheophytin a 14.26
                                                                                                           2-Pyrazolin-5-one, 4-(4'-diethylaminophenyl)imino-3-methyl-1-
Phosphine, triphenyl- 15.27
                                                                                                                              phenyl- 9.21
Phosphite, tricyclohexyl- 15.26
                                                                                                           2-Pyrazolin-5-one, 4-(4'-dimethylamino-3',5'-dimethylphenyl)imino-3-
Phosphite, triethyl- 15.24
                                                                                                                              methyl-1-phenyl- 9.19
Phosphite, trimethyl- 15.23
                                                                                                           2-Pyrazolin-5-one, 4-(4'-dimethylamino-phenyl)imino-3-methyl-1-
1,4-Phthalazinedione, 5-amino-2,3-dihydro- 7.20
Pigment from Sarcina lutea, mutant 7 2.122
                                                                                                                              phenyl- 9.18
Pigment from Sarcina lutea, mutant 93a 2.118 2.120
                                                                                                           2-Pyrazolin-5-one, 4-(4'-dimethylamino-2',3',5',6'-
Pigment from Sarcina lutea, wild-type strain 2.124
                                                                                                                              tetramethylphenyl)imino-3-methyl-1-phenyl- 9.20
Pinacyanol 9.36
                                                                                                           2-Pyrazolin-5-one, 4-(4'-diphenylaminophenyl)imino-3-methyl-1-
α-Pinene 2.74
                                                                                                                               phenyl- 9.27
β-Pinene 2.75
                                                                                                           2-Pyrazolin-5-one, 4-(4'-methoxyphenyl)imino-3-methyl-1-phenyl-
Piperazine 6.39
Piperidine 6.16
                                                                                                            2-Pyrazolin-5-one, 4,4'-[2,3,5,6-tetramethylphenylenebis]-3-methyl-1-
 Piperidine, N-(2-acetoxyethyl)-2,2,6,6-tetramethyl- 6.35
                                                                                                                               phenyl- 9.29
 Piperidine, 1-cyclohexyl- 6.36
                                                                                                            Pyridine 1.29 1a.11 5.45 79E699
 Piperidine, 2,6-dimethyl- 6.17
                                                                                                            1 \\ H- Pyrrole, \ 2-[(3,4-diethyl-5-oxo-1 \\ H-pyrrol-2-ylidene) \\ methyl]-5-methyl
 Piperidine, N-(2-hydroxyethyl)-2,2,6,6-tetramethyl- 6.34
                                                                                                                               methyl- 14.21
 Piperidine, 4-hydroxy-1,2,2,6,6-pentamethyl- 6.33
                                                                                                            Pyrrole, 2,5-dimethyl- 5.44
 Piperidine, 4-hydroxy-2,2,6,6-tetramethyl- 6.18
                                                                                                            1H-Pyrrole, 2-[(4-ethenyl-3-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-5-oxo-1H-pyrrol-2-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-3-methyl-
 Piperidine, 1-methyl- 6.32
                                                                                                                               ylidene)methyl]-4-ethyl-3,5-dimethyl- 14.17
 Porphine, tetraphenyl- 14.30
                                                                                                            1H-Pyrrole, 4-ethyl-2-[(3,4-diethyl-5-oxo-1H-pyrrol-2-
 Pregnenolone 14.12
                                                                                                                               ylidene)methyl]-3,5-dimethyl- 14.18
 Propane, 1-bromo- 1.20
                                                                                                            1H-Pyrrole, 4-ethyl-3,5-dimethyl-2-[(5-oxo-1H-pyrrol-2-ylidene)-
 Propane, 1-bromo-2,3-epoxy- 1.23
                                                                                                                                 methyl)]- 14.22
 Propane, 2-(ethylthio)-2-methyl- 11.15
                                                                                                            1H-Pyrrole, 2-[(3-ethyl-4-methyl-5-oxo-1H-pyrrol-2-ylidene)methyl]-
 Propane, 2-methyl-2-nitroso- 13.7
                                                                                                                                3,5-dimethyl- 14.19
 Propane, 2,2'-thiobis- 11.17
                                                                                                            1H-Pyrrole, 2-[(3-ethyl-4-methyl-5-oxo-1H-pyrrol-2-ylidene)methyl]-
 Propane, 2,2'-thiobis(2-methyl- 11.22
                                                                                                                                4,5-dimethyl- 14.20
 Propanoic acid, 4-hydroxy-3,5-di(2-methyl-2-propyl)phenyl ester 4.23
                                                                                                            Pyrrole, 1-(2-methyl-2-propyl)- 5.41
 2-Propanol 1.19 15.5
                                                                                                            Pyrrole, 2-(2-methyl-2-propyl)- 5.42
 2-Propanol, 2-methyl- 1.25 15.7
                                                                                                            Pyrrole, 3-(2-methyl-2-propyl)- 5.43
 2-Propenal 2.22
                                                                                                            Pyrrole, tetrahydro- 6.15
 Propene, 1-cyclopropyl-2-methyl- 2.23
                                                                                                            Pyrrolidine 6.15
 Propene, 1-cyclopropyl-2-methyl-1-phenyl- 3.20
                                                                                                            Pyrrolidine, 1-methyl-2-(3-pyridyl)- 6.30
 Propene, 1,1-dicyclopropyl- 2.24
                                                                                                            \Delta^1-Pyrroline-N-oxide, 2,4,4-trimethyl- 13.6
 Propene, 1,1-dicyclopropyl-2-methyl- 2.25
                                                                                                            \Delta^{1}-Pyrroline-N-oxide, 4.5.5-trimethyl- 13.5
 Propene-d<sub>6</sub>, 1,1-dicyclopropyl-2-methyl- 2.26
                                                                                                            Pyrylium, 2,3,2',3'-bis(1,4,10,13-trideca-4,6,8,10-tetraen)tetrayl-[4,6-
 Propene, 2-methyl- 2.21
                                                                                                                                diphenyl-, perchlorate 9.54
                                                                                                            Quinoline 5.47
 Propionitrile, 3-(N,N-diethylamino)- 6.26
 Propylamine 6.2
                                                                                                            Quinoline, poly(2,2,4-trimethyl-1,2-dihydro)- 5.48
 2-Propylamine 6.3
                                                                                                            Quinuclidine 6.38
 2-Propylamine, N-N-di(2-hydroxyethyl)-2-methyl- 6.29
                                                                                                            11-cis-Retinal 79F463
 Propylamine, 2-methyl- 6.5
                                                                                                            13-cis-Retinal 79F463
 2-Propylamine, 2-methyl- 6.6
                                                                                                            Retinal (all trans) 79F463
 Propylamine, 3-phenyl- 6.10
                                                                                                            Retinol (all trans) 2.119
 Protochlorophyll 14.24
                                                                                                            Retinyl acetate 79F463
 Protopheophytin 14.27
                                                                                                            Rubrene 3.63
 4H-Pyran, 2,3-dihydro- 15.12
                                                                                                            Ruthenium(II), tris(2,2'-bipyridine)-, dichloride 10.45
 4H-Pyran-2-t, 2,3-dihydro-4,4-dimethyl- 15.17
                                                                                                            Salicylic acid, 4-(1,1,3,3-tetramethylbutyl)phenyl ester 4.2
 4H-Pyran-3-t, 2,3-dihydro-4,4-dimethyl- 15.18
                                                                                                            Sarcina phytoene 2.118
 4H-Pyran-2-t, 2,3-dihydro-4-methyl- 15.13
                                                                                                            Sarcina phytofluene 2.120
 4H-Pyran-3-t, 2,3-dihydro-4-methyl- 15.14
                                                                                                            Sitosteryl acetate 14.14
 4H-Pyran-4-d, 2,3-dihydro-4-methyl- 15.15
                                                                                                            Stearic acid, methyl ester 14.4
 4H-Pyran-4-t, 2,3-dihydro-4-methyl- 15.16
                                                                                                            Stigmasteryl acetate 14.13
 4H-Pyran-4-thione 11.32
                                                                                                            Stilbene (cis) 3.21
 4H-Pyran-4-thione, 2,6-dimethyl- 11.33
                                                                                                            Stilbene, 1,2-dimethoxy- 3.24
 4H-Pyran-4-thione, 2,6-diphenyl- 11.34
                                                                                                            Stilbene, a-methyl- (cis) 3.22
 4H-Pyrazole, tetramethyl- 79F278
                                                                                                            Stilbene, a-methyl- (trans) 3.23
 2-Pyrazolin-5-one, 4-(4'-aminophenyl)imino-3-methyl-1-phenyl-
                                                                                                            Styrene 3.6
                                                                                                            Styrene, m-chloro-\alpha, \beta, \beta-trimethyl- 3.11
 2-Pyrazolin-5-one, 4-(4'-amino-2',3',5',6'-tetramethylphenyl)imino-3-
                                                                                                            Styrene, p-chloro-\alpha, \beta, \beta-trimethyl- 3.12
                                                                                                            Styrene, m-cyano-\alpha, \beta, \beta-trimethyl- 3.15
                     methyl-1-phenyl- 9.17
  2-Pyrazolin-5-one, 4-(4'-diethylamino-2',6'-dimethylphenyl)imino-3-
                                                                                                            Styrene, p-cyano-\alpha, \beta, \beta-trimethyl- 3.16
                     (benzoyl-amino)-1-phenyl- 9.26
                                                                                                            Styrene, \alpha-cyclopropyl-\beta,\beta-dimethyl- 3.20
  2-Pyrazolin-5-one, 4-(4'-diethylamino-2',6'-dimethylphenyl)imino-3-
                                                                                                            Styrene, p-(N,N-\text{dimethylamino})-\alpha,\beta,\beta-\text{trimethyl}- 3.19
                                                                                                            Styrene, m-methoxy-\alpha, \beta, \beta-trimethyl- 3.17
                      methyl-1-phenyl- 9.23
  2-Pyrazolin-5-one, 4-(4'-diethylamino-2',6'-dimethylphenyl)imino-3-
                                                                                                            Styrene, p-methoxy-\alpha,\beta,\beta-trimethyl- 3.18
                                                                                                            Styrene, \( \beta - methyl- \( (cis ) \) 3.7
                      (2-methyl-2-propyl)-1-phenyl- 9.25
                                                                                                            Styrene, \( \beta - \text{methyl- (trans) 3.8} \)
  2-Pyrazolin-5-one, 4-(4'-diethylamino-2'-methylphenyl)imino-3-
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Styrene, m-methyl- α, β, β -trimethyl- 3.14

methyl-1-phenyl- 9.22

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Styrene, p-methyl-\alpha,\beta,\beta-trimethyl- 3.13
Styrene, \alpha,\beta,\beta-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<sub>6</sub> 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
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
4H-Thiopyran-4-thione 11.43
4H-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
\delta-Tocopherol 4.25
α-Tocopheryl acetate 14.3
Toluene 1.36 79E699
4H-[1,2,4]Triazolo[1,2,a]norbornane, 4-methyl-3,5-dioxo- 5.50a
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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-d₂ 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

Recently Published References

79A106 Gorman, A.A., Lovering, G., Rodgers, M.A.J., The entropy-controlled reactivity of singlet oxygen $(^1\Delta_{\rm g})$ toward furans and indoles in toluene. A variable-temperature study by pulse radiolysis, J. Am. Chem. Soc. 101(111): 3050-5 (1979).

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

79A111 Matheson, I.B.C., The absolute value of the reaction rate constant of bilirubin with singlet oxygen in D₂O, Photochem. Photobiol. 29(5): 875-8 (1979).

bilirubin k_d - H_2O

79A112 Matheson, I.B.C., Lee, J., Chemical reaction rates of amino acids with singlet oxygen, Photochem. Photobiol. 29(5): 879-81 (1979).

> histidine tryptophan methionine tyrosine alanine

79A113 Matheson, I.B.C., Lightner, D.A., Oxodipyrromethenes as reactive singlet oxygen acceptors. Measurement of their chemical reaction rates by a laser flash photolysis technique, Photochem. Photobiol. 29(5): 933-5 (1979).

 $O_2(^3\Sigma_g)$

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

79A241 George, M.V., Kumar, Ch.V., Scaiano, J.C., Photochemistry and photooxidation of tetraphenyl-p-dioxin, J. Phys. Chem. 83(19): 2452-5 (1979).

tetraphenyl-p-dioxin

79E106 Stevens, B., Small, R.D., Jr., Solute re-encounter probabilities from dissociative oxciplex relaxation, Chem. Phys. Lett. 61(2): 233-8 (1979).

1,3-diphenylisobenzofuran

79E611 Wu, K.C., Trozzolo, A.M., Production of singlet molecular oxygen from the $\rm O_2$ quenching of the lowest excited singlet state of rubrene, J. Phys. Chem. 83: 2823-6 (1979).

1,3-diphenylisobenzofuran

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

 $\begin{array}{c} k_{\rm d}{-}{\rm CCl_4} \\ k_{\rm d}{-}{\rm CHCl_3} \\ k_{\rm d}{-}{\rm C_6H_6} \\ k_{\rm d}{-}{\rm C_6H_5CH_3} \\ k_{\rm d}{-}({\rm CH_3})_2{\rm CO} \\ k_{\rm d}{-}{\rm C_5H_5N} \\ k_{\rm d}{-}({\rm CH_3CH_2})_2{\rm O} \\ k_{\rm d}{-}{\rm CH_3CH_2OH} \end{array}$

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

79F118 Norris, R.D., Lightner, D.A., On the photooxygenation and autoxidation of dipyrrylmethenes and dipyrrylmethanes, J. Heterocycl. Chem. 16(2): 263-72 (1979).

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 (¹O₂) 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 $^{1}O_{2}$ 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-cyclodecylidene-ethanol
2-cycloddecylidene-ethanol
(E)-3-methyl-2-pentenol
(E)-3,7-dimethylocta-2,7-dienol
(E)-3,4-dimethyl-2-octenol
(E)-3,4-dimethyl-2-octenol
(E)-3,4-dimethyl-2-pentenol
(E)-3,4-dimethyl-2-pentenol
(E)-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).

 $\begin{array}{c} \it cis\text{-} tetramethylethylene-d_6\\ \it trans\text{-} tetramethylethylene-d_6\\ \it 2\text{-} methyl-2\text{-} pentene-4d \end{array}$

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., Photooxidation of azines. Evidence for a free-radical oxidation initiated by singlet oxygen, J. Am. Chem. Soc. 101(17): 5106-7 (1979).

acetone azine tetramethyl-4H-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).

 $1,3\text{--diphenylisobenzofuran} \\ N_3^- \ \ \text{in dodecylammonium propionate micelles}$

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).

 $k_{
m d}$ -H $_2$ O(micelles) $k_{
m d}$ -D $_2$ O(micelles) 1,3-diphenylisobenzofuran(micelles)

Appendix I

Appendix II

A More Complete Kinetic Scheme

In the kinetic scheme shown in figure 1, S = Sensitizer, ${}^{1}S^* = Excited singlet state$, ${}^{3}S^* = Excited triplet state$, 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 |
|---|--|---------------------------------------|
| $^{1}S + h\nu \rightarrow ^{1}S^{*}$ | Absorption (Rate $=I_a$) | |
| $^{1}S^{*} \rightarrow ^{1}S_{0} + h\nu$ | Fluroescence of ¹ S* | k_{F} |
| ${}^{1}S^{*} \rightarrow {}^{1}S_{0}$ | Radiationless decay of ¹ S* | $k_{ m Sd}$ |
| $^{1}S^{*} + Q \rightarrow ^{1}S_{0} + Q$ | Quenching of ¹ S* by Q | $k_{\mathrm{Sd}}{}^{\mathrm{Q}}$ |
| $^{1}\mathrm{S^{*}}\ +\ ^{3}\mathrm{O}_{2}\ \rightarrow\ \mathrm{products}$ | Reaction of ¹ S* with O ₂ | $k_{\mathrm{Sr}}^{-\mathrm{O}2}$ |
| ${}^{1}S^{*} + A \rightarrow products$ | Reaction of ¹ S* with A | $k_{\mathrm{Sr}}^{}\mathrm{A}}$ |
| $^{1}S^{*} \rightarrow {}^{3}S^{*}$ | Intersystem Crossing from ¹ S* | \pmb{k}_{ise} |
| ${}^{1}S^{*} + Q \rightarrow {}^{3}S^{*} + Q$ | Catalyzed intersystem crossing by Q | $k_{ m isc}^{-Q}$ |
| ${}^{1}S^{*} + {}^{3}O_{2} \rightarrow {}^{3}S^{*} + {}^{3}O_{2}$ | Catalyzed intersystem crossing by O ₂ . | k_{isc}^{02} |
| ${}^{1}S^{*} + {}^{3}O_{2} \rightarrow {}^{3}S^{*} + {}^{1}O_{2}^{*}$ | Energy transfer from ¹ S* to give ¹ O ₂ * and ³ S* | $k_{ m S\Delta}^{ m \ O2}$ |
| $^{3}S^{*} \rightarrow ^{1}S$ | Decay of ³ S* | k_{Td} |
| ${}^{3}S^{*} + Q \rightarrow {}^{1}S + Q$ | Catalyzed triplet decay by Q | $k_{\mathrm{Td}}{}^{\mathrm{Q}}$ |
| ${}^{3}S^{*} + {}^{3}O_{2} \rightarrow {}^{1}S + {}^{3}O_{2}$ | Catalyzed triplet decay by ${\rm O}_2$ | $k_{\mathrm{Td}}^{-\mathrm{O}_2}$ |
| $^3S^* + ^3O_2 \rightarrow products$ | Reactions of ${}^3S^*$ with O_2 | $k_{\mathrm{Tr}}^{2}}$ |
| $^3S^* + A \rightarrow products$ | Reaction to ³ S* with A | $k_{\mathrm{Tr}}^{}\mathrm{A}}$ |
| ${}^{3}S^{*} + {}^{3}O_{2} \rightarrow {}^{1}S + {}^{1}O_{2}^{*}$ | Energy transfer from ${}^3S^*$ to give ${}^1O_2^*$ | $k_{\mathrm{T}\Delta}^{\mathrm{O}_2}$ |
| $^{1}O_{2}^{*} \rightarrow {}^{3}O_{2}$ | Decay of singlet oxygen | k_{d} |
| $^{1}O_{2}^{*} + A \rightarrow \text{products}$ | Reaction of ${}^{1}O_{2}^{*}$ with A | k_r^{A} |
| $^{1}O_{2}^{*} + A \rightarrow ^{3}O_{2} + A$ | Physical Quenching of ${}^{1}O_{2}^{*}$ by A | $k_{ m q}^{\;\;A}$ |
| ${}^{1}O_{2}^{*} + Q \rightarrow {}^{3}O_{2} + Q$ | Physical Quenching of ${}^{1}O_{2}^{*}$ by Q | $k_{\eta}^{\ Q}$ |
| $^{1}O_{2}^{*} + Q \rightarrow products$ | Reaction of ¹ O ₂ * with Q | $k_{\rm r}^{\ m Q}$ |

Global Adjustment of Second Order Rate Constants²

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, 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.

²The 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 $\langle k^{A} \rangle$ 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 $10^{2\times 0.298} \approx 4$).

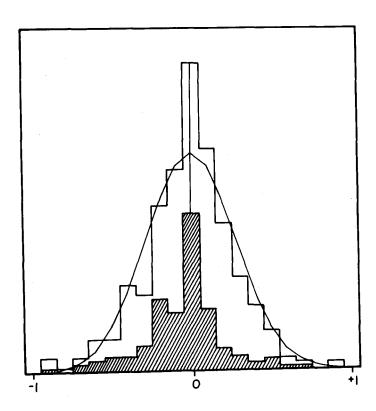


FIGURE 3. Histogram of relative deviations between measured values of k_r and the values $\langle k_r \rangle$ selected to give the least square fit to all of the measured values. The intervals are of size 0.1 in $\log_{10}(k_r/\langle k_r \rangle)$, the full range being from -1.0 to +1.0 covers a factor 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 $\langle k_{\rm r} \rangle$ 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 >

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 diphenylisobenzo-furan 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 H2O, 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 | $\langle k_{\rm r} \rangle^{\rm a} / { m dm}^3 \ { m mol}^{-1} \ { m s}^{-1}$ | 95% ^b | N^{c} |
|------------------------------|---|------------------|---------|
| | | | |
| 2.1 ^d | 7.03 × 10⁴ | 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 5 |
| 2.59 | 1.10×10^{5} 1.90×10^{5} | >10.00 | |
| 2.64 | 1.90×10^{5} 1.02×10^{5} | | 2 |
| 2.0 4 2.71 | 1.02×10^{5} 1.20×10^{5} | >10.00 | 2 |
| 2.7 1 2.7 4 | 2.03×10^4 | 2.98 | 4 |
| | 4.90×10^4 | 1.77 | 8 |
| 2.75 | | 5.9 | 3 |
| 2.86 | 3.00×10^{7} 2.00×10^{6} | 2.34 | 5 |
| 2.90 2.91 | | 1.89 | 7 |
| | 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 |
| 1.7 | 2.55×10^6 | 2.98 | 4 |
| 1.9 | 8.11×10^{5} | >10.00 | 2 |
| 1.12 | 1.09×10^6 | 5.49 | . 3 |
| 1.28 | 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 |
| 1.17 | 8.07×10^{9} | >10.00 | 2 |
| 0.1 | 5.89×10^{8} | 1.77 | 8 |
| 0.4 | 3.46×10^{8} | 2.98 | 4 |
| 0.6 | 5.56×10^{7} | 2.34 | 5 |
| 1.45 | 9.78×10^{7} | >10.00 | 2 |
| 4.5 | 1.13×10^{5} | 5.49 | 3 |
| 4.6 | 1.81×10^{5} | 5.49 | 3 |
| 4.7 | 2.26×10^{5} | 2.98 | 4 |
| 4.9 | 8.44×10^{4} | 1.89 | 7 |
| 4.32 | 1.86×10^{8} | 1.69 | 9 |

Prefered value of k..

^b95% confidence limits on $\langle k_{\rm r} \rangle$.

^cNumber of k_r values included in the determination of $\langle k_r \rangle$. ^dEntry 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 | $\langle k_{\rm r} \rangle^{\rm b} /$ ${ m Im}^3 \ { m mol}^{-1} \ { m s}^{-1}$ | Average $k_r^c/$ dm ³ mol ⁻¹ s ⁻¹ | Ratiod | 95% ^e |
|------------------|----------------------|----------------|--|---|--------|------------------|
| 2.1 ^f | (Me) ₂ CO | 3 | 7.03 × 10 ⁴ | 4.74×10^{4} | 1.48 | 2.74 |
| 2.3 | (Me) ₂ CO | 4 | 3.87×10^{7} | 3.87×10^{7} | 1.00 | 1.32 |
| 2.4 | (Me),CO | 3 | 2.07×10^{7} | 2.07×10^{7} | 1.00 | 3.86 |
| 2.12 | (Me) ₂ CO | 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),CO | 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 ₃ CN | 2 | 8.13×10^{5} | 1.59×10^{6} | 1.95 | 4.93 |
| 2.40 | (Me) ₂ SO | 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),CO | 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 ₃ CN | 6 | 1.98×10^5 | 2.43×10^{5} | 1.23 | 2.12 |
| 2.56 | (Me) ₂ CO | 2 | 1.98×10^{5} | 4.17×10^{5} | 2.10 | >100. |
| 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 | МеОН | 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 ₃ CN | 2 | 1.02×10^5 | 1.02×10^5 | 1.00 | > 100.0 |
| 2.71 | CH ₃ CN | 4 | 1.20×10^{5} | 1.02×10^{5} 1.20×10^{5} | 1.00 | 4.29 |
| 2.74 | CH ₃ CN | 2 | 2.03×10^4 | 2.14×10^{4} | 1.06 | >100.0 |
| 2.74 | MeOH | 6 | 2.03×10^{4} 2.03×10^{4} | 1.99×10^4 | 1.02 | 1.52 |
| 2.75 | CH ₃ CN | 2 | 4.90×10^{4} | 3.43×10^4 | 1.02 | 3.22 |
| 2.86 | MeOH | 2 | 3.00×10^7 | 2.35×10^{7} | 1.43 | 1.30 |
| 2.86 | X | 3 | 3.00×10^{7} 3.00×10^{7} | 3.53×10^{7} | 1.18 | 3.68 |
| 2.90 | MeOH | 2 | 2.00×10^{6} | 3.33×10^{6} 3.33×10^{6} | 1.18 | |
| 2.90 | X | 2 | 2.00×10^{6} 2.00×10^{6} | 3.84×10^6 | | > 100. |
| 2.91 | MeOH | 5 | 3.49×10^{6} | | 1.92 | >100. |
| 2.91 | X | 2 | J.47 X 10 | 3.09×10^{6} | 1.13 | 2.42 |

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

| Substrate | Solvent | Nª | $\langle k_{\rm r} \rangle^{\rm b} /$ dm ³ mol ⁻¹ s ⁻¹ | Average k_r^c / dm ³ mol ⁻¹ s ⁻¹ | Ratiod | 95% ^e |
|--------------|---|-----|--|--|--------|------------------|
| 2.130 | C ₆ H 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 ₃ CN | 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 | CCl₄ | 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 | CCl₄ | 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 ₂ O | 4 | 2.33×10^{8} 2.33×10^{8} | 1.13×10^{9} | 4.86 | 2.38* |
| 5.29 | MeOH | 5 | 2.33×10^{8} 2.33×10^{8} | 2.89×10^{8} | 1.24 | 2.09 |
| 5.29 | X | 4 | 2.33×10^{8} 2.33×10^{8} | 1.24×10^8 | 1.87 | 5.30 |
| 5.30 | C ₆ H 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 ₃ CN | 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) ₂ CO | 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,H,N | 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,Cl, | 4 | 6.34×10^{8} | 8.58×10^{8} | 1.35 | 1.84 |
| | | 3 | 6.34×10^{8} | 1.36×10^{9} | 2.15 | 73.30 |
| 5.36 | CH ₃ CN | 5 | 6.34×10^{8} 6.34×10^{8} | 4.91×10^{8} | 1.29 | 2.10 |
| 5.36 5.36 | CHCl ₃ | 3 | 6.34×10^{8} | 9.32×10^{8} | 1.47 | 1.76 |
| 5.36 | dioxane | 3 | 6.34×10^{8} 6.34×10^{8} | 8.31×10^{8} | 1.31 | 4.05 |
| 5.36 | EtOH | | 6.34×10^{8} 6.34×10^{8} | 8.87×10^9 | 13.98 | 3.23* |
| 5.36 5.36 | H ₂ O | 5 | 6.34×10^{8} 6.34×10^{8} | | 1.62 | 9.36 |
| 5.36 | i-PrOH | 3 | | 3.92×10^8 | 1.02 | 1.25 |
| 5.36 | (Me) ₂ CO | 3 | 6.34×10^8 | 6.21×10^8 | | |
| 5.36 | C ₆ H ₅ CH 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 | Nª | $\langle k_{\rm r} \rangle^{\rm b} /$ dm ³ mol ⁻¹ s ⁻¹ | Average k_r^c / dm ³ mol ⁻¹ s ⁻¹ | Ratio ^d | 95% ^e |
|-----------|---------------------------------|-----|--|--|--------------------|------------------|
| 9.1 | CH ₃ CN | 4 | 5.89 × 10 ⁸ | 6.46×10^{8} | 1.10 | 2.01 |
| 9.1 | CHCl, | 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 ₃ CN | 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 ₅ H ₅ N | 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 | >100.0 |
| 14.7 | C ₅ H ₅ N | 3 | 2.26×10^{5} | 2.07×10^{5} | 1.09 | 1.76 |
| 14.9 | C ₅ H ₅ N | 7 | 8.44×10^{4} | 8.44×10^{4} | 1.00 | 1.14 |
| 14.32 | $CC1_4$ | 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 | >100.0 |
| 14.32 | Y | 2 | 1.86×10^{8} | 1.58×10^{8} | 1.18 | >100.0 |

^aNumber of k_r values determined in this particular solvent.

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

| No.ª | Substrate | $< k_{\rm r} > {}^{\rm b} /$ dm ³ mol ⁻¹ s ⁻¹ | 95%° |
|---------------|---|---|-----------------|
| A3.1 | 2-methyl-2-butene (2M2B, 2.33)° | 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 |
| A 3.10 | 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 |
| 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 |

^aEntry numbers used in the Comments column in tables 1-15 to index preferred values of k_r .

^bPreferred value of k_r .

^cAverage value of k_r for this particular solvent.

^dRatio of Average value of k_r for this particular solvent to $\langle k_r \rangle$; ratio is inverted if less than one.

e95% confidence limits on Ratio. Only values marked with an asterisk are less than the Ratio.

Entry number in tables 2-14 where substrates are identified and reported rate data for substrates are given.

⁸Solvent X = MeOH/t-BuOH (1:1); solvent Y = other mixed solvents.

^bPreferred value of k_r .

^{°95%} confidence limits on $\langle k_r \rangle$.

^dβ(MeOH) for 2,5-diphenylfuran is calculated by taking the ratio of $k_d = *1.0 \times 10^5 \text{ s}^{-1}$ [1.3.6] to $\langle k \rangle_r = 6.98 \times 10^7 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ [43.16].

^eEntry 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 $k_{\rm r}$ 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 $\langle k_{\rm r} \rangle$ 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.