

The reactions of OH radicals with di-*i*-propoxymethane and di-*sec*-butoxymethane: Kinetic measurements and structure activity relationships

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The gas-phase reactions of OH($X^2\Pi$) radicals with di-*i*-propoxymethane (DiPM) and di-*sec*-butoxymethane (DsBM) have been studied in argon in the temperature range 295–700 K at total pressures between 50 and 400 Torr. OH radicals were generated by excimer laser photolysis of H_2O_2 and were detected by laser-induced fluorescence. Within the investigated ranges, the reactions of OH($X^2\Pi$) radicals with DiPM and DsBM were found to be independent of total pressure. Weak dependencies of the rate coefficients on temperature were observed. Bimolecular rate coefficients for the reactions of OH($X^2\Pi$) with DiPM and DsBM at 298 K of $k_{OH+DiPM} = (3.47 \pm 0.20) \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ and $k_{OH+DsBM} = (4.25 \pm 0.13) \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$, respectively, have been determined. In order to describe the kinetics of the reactions of OH radicals with DiPM and DsBM as well as analogous acetals, a structure activity relationship (SAR) technique established for other reactant classes has been modified and applied. Compared to the former SAR method, which does not yield satisfying results for oxygenated VOCs (volatile organic compounds), the present calculations lead to much better agreement with the experimental data for dialkylacetals of the type $R-O-CH_2-O-R$.

1. Introduction

In recent years the reformulation of gasoline by adding oxygenated VOCs (volatile organic compounds) has become more common. There are several advantages of using oxygenated organic compounds such as ethers and alcohols as fuel additives. These compounds enhance the octane level, increase the efficiency of combustion, and reduce the emission of atmospheric pollutants, *e.g.* hydrocarbons, CO and particles.^{1–3} The possible industrial application of a large number of new oxygenated compounds such as acetals or esters is currently under discussion.⁴ In addition, both classes of compounds are being considered as alternative solvents.

Particularly the two compounds under investigation here, di-*i*-propoxymethane (DiPM) and di-*sec*-butoxymethane (DsBM), are currently under consideration as diesel fuel components. It has been shown, that the addition of acetals with the general structure $R-O-CH_2-O-R$ to diesel fuel significantly reduces the emission of particulate matter from diesel engines.³

However, the widespread use of these organic compounds might also lead to a significant influence of these species on tropospheric chemistry. It is known that the reformulation of fuel by oxygenated VOCs increases the exhaust concentration of aldehydes.⁵ Also the discovery of several oxygenated organic compounds like methyl-*tert*-butylether (MTBE) in groundwater and reservoirs used for drinking water⁶ show the necessity to improve the knowledge about the kinetic and mechanistic behaviour of oxygenated VOCs and their reaction products in the troposphere. Detailed information about the atmospheric chemistry of such compounds is generally poor. It is highly certain, that oxygenated VOCs are mainly removed from the troposphere by reaction with OH radicals. Hence, determination of the rate coefficients for their reactions with OH as well as mechanistic studies are necessary.

In the present work, the bimolecular rate coefficients for the reactions of OH radicals with DiPM and DsBM have been studied for the first time as a function of temperature. All experiments have been carried out using the well-established pulsed excimer laser photolysis (ELP)/laser-induced fluorescence (LIF) technique. The rate coefficients were measured in argon in the temperature range 295–700 K. From the results, tropospheric lifetimes of DiPM and DsBM have been estimated. The room temperature values are compared with data of Thüner *et al.*,⁷ who obtained bimolecular rate coefficients for several dialkylacetals using the relative rate technique in a static photoreactor.

In addition, the rate coefficients for the reactions of OH with DiPM and DsBM as well as for other acetals of the type $R-O-CH_2-O-R$ were calculated using the structure activity relationship (SAR) method developed by Atkinson^{8,9} and Kwok and Atkinson.¹⁰ Since this technique does not lead to sufficient agreement between experimental and theoretical data for the treated dialkylacetals, the SAR method was modified for this class of compounds. The new approach yields more reasonable results, which are in much better agreement with the measured rate coefficients than the results of the former technique.

2. Experiment

A detailed description of the experimental set-up used in the present work can be found elsewhere.¹¹ Briefly, the focused 248 nm radiation of a Lambda Physik Compex 102 excimer laser with a pulse energy of 20–100 mJ operating at 10 Hz was used to generate OH radicals by photodissociation of H_2O_2 which was evaporated in Ar. Relative OH($X^2\Pi$) concentrations were monitored by laser-induced fluorescence using the Q_1 -branch of the $A^2\Sigma^+(v' = 1) \leftarrow X^2\Pi(v'' = 0)$ transition at 282 nm and off-resonance detection of the

$A^2\Sigma^+(v'=0) \rightarrow X^2\Pi(v''=0)$ transition at 308 nm. The probe laser was a Lambda Physik system comprising a Scanmate 1 dye laser pumped by an LPX 202 excimer laser. For monitoring OH radicals the frequency-doubled dye laser was operated with Coumarin 153 (Radiant Dyes Chemie) in methanol, yielding typical pulse energies of 0.3 mJ.

The reaction cell used in the present work consisted of a cylindric stainless steel housing incorporating a ceramic cylinder. The ceramic cylinder was heated by means of a tantalum resistive wire. The temperature in the reaction cell was measured directly under the observation zone by shielded, calibrated thermocouples and kept constant during the experiments to better than ± 1.5 K. A more detailed description of the reaction cell is given elsewhere.^{12,13}

The OH fluorescence was observed perpendicular to the laser beam through a lens system and an interference filter with a photomultiplier (EMI 9635QB). The output signal of the photomultiplier was integrated by a boxcar averager (SRS model SR 250), digitised and analysed by an ATARI MegaST microcomputer equipped with a Rhotron AD transformer. The time delay between the photolysis laser and the probe laser was varied from zero to several milliseconds by means of a digital delay generator (BNC 7010). The highest time resolution used was 1 μ s.

The reactions of OH radicals with DiPM and DsBM were investigated under pseudo-first-order conditions with reactant concentrations at least a hundred times larger than the OH precursor H_2O_2 . All measurements were performed using slow flowing gas mixtures with flow rates < 0.5 m s⁻¹. The concentrations of the gases were determined from their partial flows measured by calibrated flow meters (Tylan FM 360). In all experiments argon was used as bath gas. DiPM and DsBM were diluted in argon with ratios of about 1:1000 and 1:2000, respectively, and stored in stainless steel cylinders. The exact mixing ratios of the mixtures used were determined by Fourier transform infrared spectroscopy.

Argon with a stated purity of 99.998% employed in this work was supplied by Messer-Griesheim. DiPM and DsBM (Lambiotte & Cie) were distilled twice for purification and carefully degassed before use. H_2O_2 (Peroxid-Chemie, 85 wt.%, stabilised) was used without further purification.

3. Results and discussion

3.1. Measurement of rate coefficients

From the LIF measurements, relative OH($X^2\Pi$) radical concentrations were measured as a function of the reaction time. As shown in Fig. 1, taking DiPM as an example, the LIF signal decayed exponentially for all reactant concentrations. In the absence of DiPM or DsBM, the OH decay was mainly caused by reaction with H_2O_2 . This is supported by the fact that the measured decay constants were strongly dependent on the H_2O_2 concentration.

The OH decay could be monitored over at least 3 lifetimes. The addition of DiPM or DsBM caused a more rapid decay of OH radicals. By plotting the logarithm of the relative OH concentration as a function of reaction time, pseudo-first-order decay constants k' were calculated from the slope of the individual straight line plots for different concentrations of DiPM or DsBM. The k' values increased proportionally with the concentration of the added reactant. The bimolecular rate coefficients $k_{OH+acetal}$ for a given temperature were then obtained by plotting corrected pseudo-first-order decay constants k'_{corr} as a function of the acetal concentration, as shown in Fig. 2 using DiPM as an example. The k'_{corr} values were obtained by subtracting the decay constants, which were measured in the absence of the reactant, from the corresponding k' values.

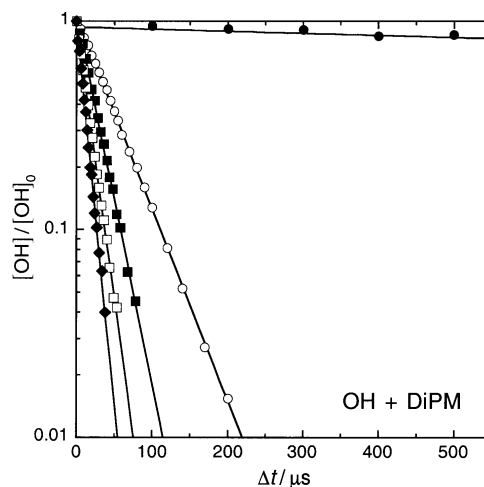


Fig. 1 Semi-logarithmic plot of the OH decay after laser photolysis of H_2O_2 at 295 K in 399 Torr Ar in the presence of different DiPM concentrations ($\times 10^{14}$ cm⁻³): (●) 0; (○) 0.51; (■) 1.01; (□) 1.56; (◆) 2.10.

Almost all studies were carried out at a total pressure of 400 Torr. A few additional experiments at total pressures of 50 and 160 Torr at room temperature yielded similar results, indicating that the reactions of OH radicals with DiPM or DsBM are independent of total pressure within this pressure range. Accordingly, rate coefficients for each reaction obtained at different total pressures for similar temperatures were averaged for further analysis of the data.

The bimolecular rate coefficients for the reaction of OH radicals with DiPM and DsBM were measured in the temperature range 295–700 K. The rate coefficients obtained for both reactions are summarised in Table 1. The error limits represent a 90% confidence interval and reflect the statistical precision only. The given rate coefficients are weighted by means of at least five k -values which were determined in independent measurements using at least 5 different acetal concentrations.

The Arrhenius plots for $k_{OH+DiPM}$ and $k_{OH+DsBM}$ are illustrated in Fig. 3 and 4, respectively. Both plots exhibit minima of the bimolecular rate coefficients at about 500 K. To higher and to lower temperatures, the rate coefficients slightly increase. This behaviour is in agreement with previous observations of Dagaut *et al.*,¹⁴ Porter *et al.*¹⁵ and Becker *et al.*,¹⁶ who investigated the reactions of OH with several acetals of the general structure of R–O–CH₂–O–R. All these reactions show only weak temperature dependencies with small activa-

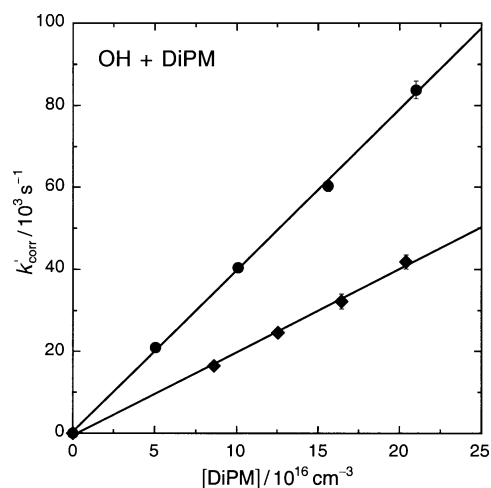


Fig. 2 Plot of pseudo-first-order decay constants k'_{corr} vs. the concentration of DiPM for 295 (●) and 500 K (◆) at 399 Torr total pressure.

Table 1 Bimolecular rate coefficients for the reaction of OH radicals with DiPM and DsBM

Reaction	T /K	k_{exp}^a / $10^{-11} \text{ cm}^3 \text{ s}^{-1}$ (this work)	k_{SAR}^b / $10^{-11} \text{ cm}^3 \text{ s}^{-1}$ (this work)	k_{SAR}^c / $10^{-11} \text{ cm}^3 \text{ s}^{-1}$ (ref. 10)
OH + DiPM	296 ± 3	3.47 ± 0.20	3.51	9.93
	350 ± 4	2.81 ± 0.12	2.62	6.69
	410 ± 2	2.22 ± 0.10	2.26	5.27
	503 ± 2	2.32 ± 0.20	2.06	4.14
	602 ± 7	3.17 ± 0.33	2.16	3.87
	697 ± 1	3.43 ± 0.08	2.41	3.94
OH + DsBM	295 ± 1	4.25 ± 0.13	4.59	11.20
	401 ± 1	2.82 ± 0.24	2.88	5.87
	501 ± 5	2.15 ± 0.38	2.68	4.76
	602 ± 4	2.56 ± 0.22	2.87	4.57
	700 ± 5	2.70 ± 0.43	3.23	4.76

^a k_{exp} = data measured in the present work (errors reflect a 90% confidence interval). ^b k_{SAR}^* = data obtained by modified SAR (this work).

^c k_{SAR} = data obtained by SAR using the method of Kwok and Atkinson.¹⁰

tion energies close to zero. Porter *et al.*¹⁵ suggested that the slight curvature of the Arrhenius plots for the reactions of OH with acetals is caused by different rate coefficients for OH attack at the different sites of the acetal. On the other hand, the negative temperature dependence of both reactions investigated in the present work might be due to the formation of a transition state including a five-membered ring for the OH attack, as proposed by Porter *et al.*¹⁵ Such a transition state is

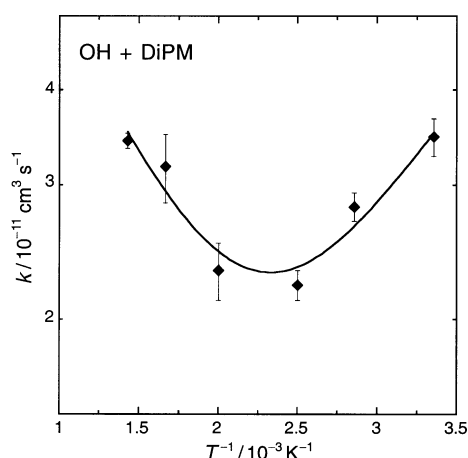


Fig. 3 Arrhenius plot of the bimolecular rate coefficient $k_{\text{OH}+\text{DiPM}}$ vs. $1/T$. (◆) experimental data (errors reflect a 90% confidence interval). The solid line is a fit corresponding to eqn. (1).

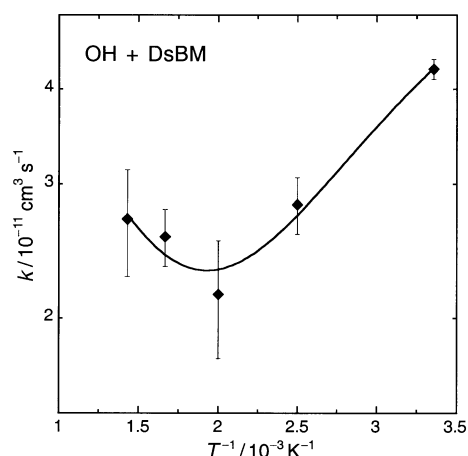


Fig. 4 Arrhenius plot of the bimolecular rate coefficient $k_{\text{OH}+\text{DsBM}}$ vs. $1/T$. (◆) experimental data (errors reflect a 90% confidence interval). The solid line is a fit corresponding to eqn. (2).

possible for OH attack to both CH_x groups connected directly to one of the O atoms, which is schematically illustrated in Fig. 5. The stability of the proposed structure will decrease with increasing temperature. As a consequence, the rate coefficient of the corresponding reaction will decrease. Above a given temperature, the reaction will proceed as a typical abstraction reaction and the rate coefficient will exhibit a positive temperature dependence. Taking into account that for all acetals currently investigated, more than about 90% of the OH radicals attack H atoms in α position to one of the oxygen atoms,¹⁷ this might explain the presently observed minima in the Arrhenius plots of $k_{\text{OH}+\text{DiPM}}$ and $k_{\text{OH}+\text{DsBM}}$ and the increase of the rate coefficients at higher temperatures.

The temperature dependencies of $k_{\text{OH}+\text{DiPM}}$ and $k_{\text{OH}+\text{DsBM}}$ are well described by the following biexponential expressions obtained by weighted non-linear least squares procedures using the inverse squares of experimental errors of the rate coefficients as statistical weight:

$$k_{\text{OH}+\text{DiPM}} = (2.14^{+0.63}_{-0.27}) \times 10^{-12} \times \exp[(812^{+168}_{-82})/T] \\ + (1.76^{+0.22}_{-0.17}) \times 10^{-10} \times \exp[-(1275^{+55}_{-70})/T] \quad (1)$$

$$k_{\text{OH}+\text{DsBM}} = (6.22^{+0.58}_{-0.60}) \times 10^{-12} \times \exp[(572^{+52}_{-50})/T] \\ + (3.13^{+0.57}_{-0.08}) \times 10^{-10} \times \exp[-(2205^{+15}_{-95})/T] \quad (2)$$

as illustrated in Fig. 3 for $k_{\text{OH}+\text{DiPM}}$ and in Fig. 4 for $k_{\text{OH}+\text{DsBM}}$.

The results of the present work of $k_{\text{OH}+\text{DiPM}} = (3.47 \pm 0.20) \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ and $k_{\text{OH}+\text{DsBM}} = (4.25 \pm 0.13) \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ at room temperature are in good agreement with data of Thüner *et al.*,⁷ who determined $k_{\text{OH}+\text{DiPM}} = (3.93 \pm 0.48) \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ and $k_{\text{OH}+\text{DsBM}} = (4.68 \pm 0.05) \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ by using the relative rate technique in a static photo-reactor.

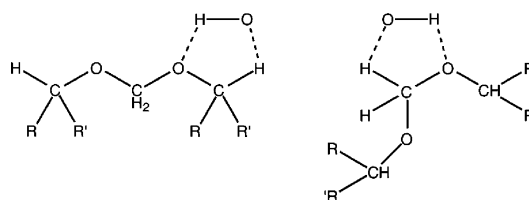


Fig. 5 Schematic structures of possible transition states for OH attack to acetals of the type $\text{R}-\text{O}-\text{CH}_2-\text{O}-\text{R}$ in α -position to the central CH_2 group.

Table 2 Comparison of bimolecular rate coefficients for the reactions of OH radicals with selected acetals of the type R–O–CH₂–O–R at room temperature

Compound	k_{SAR}^a / 10^{-11} cm ³ s ⁻¹ (this work)	k_{SAR}^b / 10^{-11} cm ³ s ⁻¹ (ref. 10)	k_{exp}^c / 10^{-11} cm ³ s ⁻¹	Refs. (k_{exp})
Dimethoxymethane	0.41	6.82	0.49 ± 0.08	15
Diethoxymethane	1.78	8.19	2.04 ± 0.14	15
di-n-butoxymethane	2.65	9.07	3.39 ± 0.46	16
di-i-propoxymethane	3.51	9.93	3.47 ± 0.20	This work
di-sec-butoxymethane	4.50	10.91	4.25 ± 0.13	This work

^a k_{SAR}^a = data obtained by modified SAR (this work). ^b k_{SAR}^b = data obtained by SAR using the method of Kwok and Atkinson.¹⁰ ^c k_{exp} = experimental data.

From the bimolecular rate coefficients $k_{\text{OH}+\text{DiPM}}$ and $k_{\text{OH}+\text{DsBM}}$ obtained in this work, the atmospheric lifetimes of DiPM and DsBM can be estimated. It is assumed that the only significant sink of these compounds in the troposphere is reaction with OH radicals. Hence, at an OH daytime concentration of 5×10^6 cm⁻³,¹⁸ typical for a summer day in a polluted region, the atmospheric lifetimes of DiPM and DsBM at 298 K are (1.6 ± 0.1) h and (1.3 ± 0.1) h, respectively.

These relatively short lifetimes indicate that DiPM and DsBM will be removed rapidly during daylight from the troposphere. As a consequence, the products of the OH-initiated oxidation of DiPM and DsBM could possibly contribute to local photochemical formation. Therefore, intensive mechanistic and product studies on this compound should be carried out in the near future to assess the ozone forming potential of these compounds.

3.2. Structure activity relationship (SAR) calculations

In addition to the kinetic measurements, the rate coefficients measured in the present work have been compared with estimations obtained using the structure activity relationship (SAR) algorithm by Atkinson^{8,9} and Kwok and Atkinson.¹⁰ Table 1 summarises all experimentally obtained rate coefficients

for the reactions of OH with DiPM and DsBM in comparison to those calculated using the SAR method. All reaction rate coefficients calculated using the technique of Kwok and Atkinson¹⁰ are evidently larger than the measured values. For both compounds the deviations increase with decreasing temperature. In the present work, significant modifications of the established SAR technique were made in order to achieve better agreement of experimental and SAR data for the investigated acetals and other compounds of this reactant class. Using the original SAR method,^{8–10} bimolecular rate coefficients for the reactions of OH radicals with organic compounds are determined as follows. Briefly, OH radical reactions with organic compounds proceed by four different reaction pathways. H-atom abstraction, OH radical addition to multiple C–C bonds, OH radical addition to aromatic rings and OH radical interaction with N-, S- or P-atoms. The four reaction pathways are assumed to be additive. The investigated reactions of acetals with OH only proceed by H-atom abstraction. In order to calculate the overall rate coefficient, the group rate coefficients k_{prim} , k_{sec} , and k_{tert} for the groups –CH₃X, –CH₂XY and –CHXYZ, where X, Y and Z are substituents, have to be determined. The different substituents are considered by the substituent factors $F(X)$, $F(Y)$ and $F(Z)$. The individual groups are calculated by multiplication of the group rate constants with the substituent factors and the total rate constant is given by the addition of all groups.

This technique generally works well for mono-substituted organic compounds. The acetals investigated in this study show a rather poor agreement between the experimental data and the calculated values, as shown in Table 1. Most of the calculated rate coefficients disagree by more than a factor of 3 within the experimental values.

In the present work, the group rate constant for the central CH₂ group of the acetals was not calculated as proposed by Kwok and Atkinson¹⁰ by multiplying the mono-substituent factor $F(\text{O-alkyl})$ by two. Here, a new double-substituent factor $F[(\text{O-alkyl})_2]$ was defined. Kwok and Atkinson¹⁰ give a substituent factor $F_{298}(\text{O-alkyl})$ of 8.4. The new double-substituent factor $F_{298}[(\text{O-alkyl})_2]$ was set to 1.9, which leads to a group rate constant of a factor of about 8 smaller than recommended by Kwok and Atkinson¹⁰ for the central CH₂ group.

The new double-substituent factor was obtained by analysing all available data for compounds of the type R–O–CH₂–O–R, including absolute rate coefficients and their temperature dependencies as well as the branching ratios of the OH attack at each compound. Variation of the factor and comparison of calculated and experimental data yielded 1.9 as the best value for $F[(\text{O-alkyl})_2]$. Table 2 compares the experimental rate coefficients for room temperature with those obtained using the modified SAR technique from this work and also the values obtained using the strategy of Kwok and Atkinson.¹⁰ Most of the rate coefficients calculated using the modified SAR disagree by only $\pm 20\%$ with the experimental values.

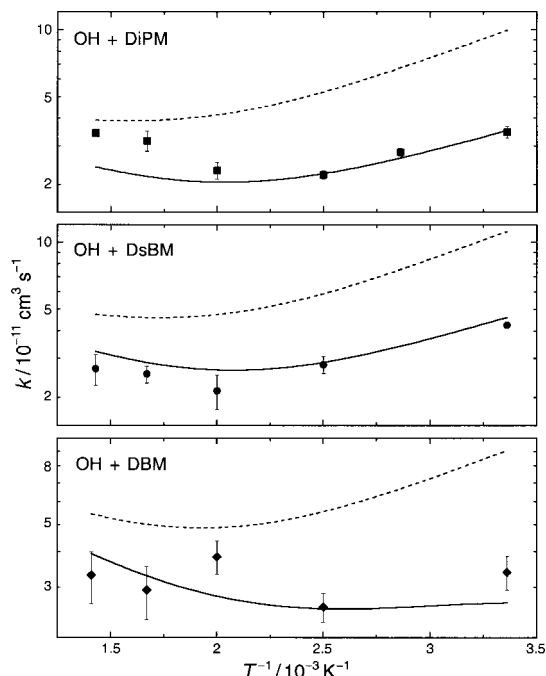


Fig. 6 Arrhenius plots for the reactions of OH radicals with selected acetals. Experimental data: DiPM (■) (this work), DsBM (●) (this work), DBM (◆) (ref. 16); SAR calculations: (—) (this work), (---) (ref. 10).

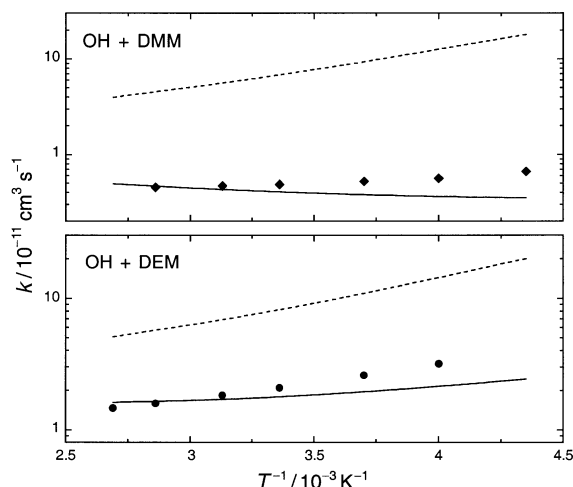


Fig. 7 Arrhenius plots for the reactions of OH radicals with selected acetals. Experimental data: DMM (◆) (ref. 15), DEM (●) (ref. 15); SAR calculations: (—) (this work), (---) (ref. 10).

Calculations of the temperature dependencies of the bimolecular rate coefficients for compounds of the general structure $R-O-CH_2-O-R$ using the presently defined double substituent factor $F[(O-alkyl)_2]$ also yield significantly better agreement of calculated and experimental data than the original description of Kwok and Atkinson,¹⁰ as illustrated in Fig. 6 for DiPM, DsBM and di-*n*-butoxymethane (DBM) and in Fig. 7 for dimethoxymethane (DMM) and diethoxymethane (DEM). The experimental data for DiPM and DsBM were determined in the present work (see Table 1), the measured rate coefficients for DMM and DEM were obtained by Porter *et al.*,¹⁵ the experimental data for DBM were measured by Becker *et al.*¹⁶ For all compounds, the SAR results calculated using the parameters of Kwok and Atkinson¹⁰ (dashed lines in Figs. 6 and 7) are significantly higher than the experimental rate coefficients. The highest deviations occur for DMM, where the calculated data are at least a factor of ten higher than the measured values. Using the new double-substituent factor for the central CH_2 group of the acetals, the calculated rate coefficients (solid lines in Figs. 6 and 7) agree notably better with the measured values for all temperatures. However, the agreement between theoretical and experimental data is not of similar quality for all compounds. While excellent agreement was obtained for DsBM and DBM, the calculated data for DiPM underestimate the measured values at temperatures above 500 K, the aberration increases with increasing temperature. For DMM and DEM the calculated temperature dependence is weaker than the measured one, for temperatures below about 300 K the calculations underestimate the experimental data, resulting in an increase in deviation with decreasing temperature.

Finally, the use of the presently defined double-substituent factor $F[(O-alkyl)_2]$ in SAR calculations also leads to a better

assessment of the branching ratios for the OH reaction channels with acetals of the general structure $R-O-CH_2-O-R$ compared to the classical method of Kwok and Atkinson,¹⁰ as illustrated in Table 3. The experimental data on the percentage of OH attack to the central CH_2 group of each compound were obtained from product studies by Wallington *et al.*⁴ in an indoor photoreactor and by Maurer *et al.*¹⁷ in an outdoor smog chamber. Using the double-substituent factor $F[(O-alkyl)_2]$, the ratios obtained for the OH attack at the central CH_2 group are in agreement with the measured data within the experimental errors, except for DMM, where the calculated value of 0.44 is about 50% larger than the experimentally obtained value of 0.3. The calculations performed using the original procedure of Kwok and Atkinson¹⁰ lead to ratios which are significantly higher than those obtained from the experiments.

In conclusion, the definition of a double substituent factor $F[(O-alkyl)_2]$ for SAR calculations on the OH reactions of acetals of the type $R-O-CH_2-O-R$ yields better agreement for rate coefficients and their temperature dependencies as well as for the branching ratios of the OH attack to the different reactants than the method previously defined by Atkinson^{8,9} Kwok and Atkinson¹⁰ using only single-substituent factors.

4. Summary

The reactions of $OH(X^2\Pi)$ with di-*i*-propoxymethane (DiPM) and di-*sec*-butoxymethane have been studied over the temperature range 295–700 K by excimer laser photolysis/laser-induced fluorescence. The rate coefficients were found to be independent of total pressure in the range 50–400 Torr. Within the investigated range, only a weak temperature dependence of the bimolecular rate coefficients was observed. For both compounds investigated, the Arrhenius plots exhibit positive slopes at lower and negative slopes at higher temperatures with minima at about 500 K. From the rate coefficients obtained at room temperature, the tropospheric lifetimes of DiPM and DsBM were derived.

The rate coefficients have also been compared with calculations using structure activity relationship (SAR) techniques. An established SAR method was modified in the present work, leading to significantly better agreement of experimental and theoretical rate coefficients for both temperature dependencies and branching ratios for the reactions of OH radicals with acetals of the general type $R-O-CH_2-O-R$.

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Table 3 OH-initiated oxidation of selected acetals of the type $R-O-CH_2-O-R$ at room temperature. Comparison of experimental and calculated fractions of the OH attack at the central CH_2 groups of each compound

Compound	Experimental (%)	Refs.	SAR* ^a (%) (this work)	SAR ^b (%) (ref. 10)
Dimethoxymethane	30 ± 5	4, 17	44	97
Diethoxymethane	10 ± 10	17	10	80
Di- <i>n</i> -propoxymethane	5 ± 10	17	7	75
Di- <i>n</i> -butoxymethane	10 ± 10	17	7	73
Di- <i>i</i> -propoxymethane	10 ± 10	17	5	66

^a SAR* = modified SAR data obtained in the present work. ^b SAR = SAR data obtained by the method of Kwok and Atkinson.¹⁰

DiPM and DsBM and T. Maurer, C. G. Sauer and L. P. Thüner for providing the results of their experimental work on acetals prior to publication.

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