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SO₂ formation and peroxy radical isomerization in the atmospheric reaction of OH radicals with dimethyl disulfide

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The atmospheric reaction of OH radicals with dimethyl disulfide, CH₃SSCH₃, proceeds primarily via OH addition forming CH₃S and CH₃SOH as reactive intermediates, and to a lesser extent via H-abstraction resulting in the peroxy radical CH₃SSCH₂OO in the presence of O₂. The latter undergoes a fast two-step isomerization process leading to HOOCH₂SSCHO. CH₃S and CH₃SOH are both converted to SO₂ and CH₃O₂ with near unity yields under atmospheric conditions.

Dimethyl disulfide (DMDS, CH₃SSCH₃) represents one of the important reduced-sulfur compounds within Earth's sulfur cycle. DMDS is believed to account globally for a few percent of the natural, biogenic sulfur emissions beside the main species H₂S and dimethyl sulfide (DMS, CH₃SCH₃).¹ DMDS has been identified as important emission from forest and savanna fires exceeding the DMS emission in these areas by an order of magnitude.^{2,3} The atmospheric degradation of DMDS is largely driven by its gas-phase reaction with OH radicals ultimately leading to the formation of SO₂ and probably methane sulfonic acid (MSA, CH₃SO₃H).⁴⁻⁶ Sulfuric acid (H₂SO₄), arising from the subsequent oxidation of SO₂, and MSA are important precursors for the formation and growth of natural aerosol and clouds in the boundary layer.⁷

Earlier kinetic measurements have revealed a very fast OH + DMDS reaction, close to the gas-kinetic limit, connected with a negative temperature dependence that points to preferred OH-adduct formation (1a).^{8,9} The possible H-abstraction channel (1b), dominating the similar OH + DMS reaction,¹⁰ has not been considered yet. The adduct CH₃S(OH)SCH₃ is calculated to rapidly decompose forming CH₃S and CH₃SOH (2) in agreement with previous experiments (see ESI).^{1,9}

A CH₃S formation yield of 0.28 ± 0.20 has been reported from a low pressure H₂O₂ photolysis experiment in absence of oxygen and CH₃SOH was qualitatively detected as a co-product.¹¹ CH₃S along with CH₃SOO from the reversible CH₃S + O₂ reaction (3,-3)¹² represent key intermediates for SO₂ production mainly based on the unimolecular steps (4) and (5) and the reactions with ozone (6) and (7).¹⁰

In polluted areas, also CH₃S + NO₂ → CH₃SO + NO can become important.¹⁰ In CH₃S(O)O both O atoms are bound to the sulfur, while CH₃SOO has a peroxy structure. The formation of CH₃S(O)O is the rate-limiting step for SO₂ generation.^{10,13}

SO₂ yields of 0.22 - 1.83 and MSA yields of up to 0.14 have been reported from OH + DMDS end product studies for high concentration levels (biased by DMDS photolysis).⁴⁻⁶ It has been speculated that MSA is either formed via CH₃SOH + O₂ + M → CH₃SO₃H + M or via CH₃SO₃ + CH₃SOH → CH₃SO₃H + CH₃SO.^{4,5}

Herein, we present results of mechanistic studies on OH + DMDS under close to atmospheric reaction conditions with special attention to the possible H-abstraction channel (1b) as well as to the formation of SO₂ and MSA. The experiments were conducted in the free-jet flow system at 295 ± 2 K, a pressure of 1 bar of purified air and a residence time of 7.9 s. OH radicals were produced from ozonolysis of tetramethylethylene (TME) and, alternatively, via isopropyl nitrite photolysis. Chemical ionization - atmospheric pressure interface - time-of-flight mass spectrometry (CI-API-TOF) with a series of ionization schemes was applied for product analysis.¹⁴ Results from quantum chemical calculations support the mechanistic interpretation and the assessment of ionization schemes used for product identification. (See ESI for more details.)

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First, we investigated the possible product formation starting from $\text{CH}_3\text{SSCH}_2\text{O}_2$ formed by O_2 addition to CH_3SSCH_2 in the H-abstraction channel (1b). For the structurally similar $\text{CH}_3\text{SCH}_2\text{O}_2$ obtained from $\text{OH} + \text{DMS}$, theoretical results as well as experimental findings from both the laboratory and a field study consistently revealed a rapid two-step RO_2 isomerization process resulting in $\text{HOOCH}_2\text{SSCHO}$.¹⁵⁻¹⁷ Analogously, signals consistent with the expected $\text{CH}_3\text{SSCH}_2\text{O}_2$ isomerization products, i.e. $\text{O}_2\text{CH}_2\text{SSCH}_2\text{OOH}$ and the closed-shell product $\text{HOOCH}_2\text{SSCHO}$ (Scheme 1), were detected here for the first time using iodide ionization ($\text{I}^+ \text{-CI-API-TOF}$). Theoretical calculations showed that the iodide clusters of these products are only slightly less stable than the corresponding clusters from the $\text{OH} + \text{DMS}$ reaction (see ESI). The product signals increased linearly with rising DMDS conversion, in line with the first-order kinetics of RO_2 radical isomerization steps (Fig.S1). The amount of reacted DMDS was calculated by applying a detailed reaction mechanism (see ESI). Ozonolysis of TME was used for OH radical formation in a dark reaction; however, the same product signals were also observed using isopropyl nitrite photolysis as a second OH radical source (Fig.S2). Formation of the DMDS derived RO_2 isomerization products can be explained in a way identical to that proposed for $\text{OH} + \text{DMS}$.^{15, 16}

The first RO_2 isomerization step (8) proceeds via H-abstraction from the methyl group forming $\text{O}_2\text{CH}_2\text{SSCH}_2\text{OOH}$ after O_2 addition to the formed alkyl radical position (9). In the next step (10), the newly formed RO_2 radical abstracts a H atom from the hydroperoxy methylene group resulting in an unstable di-hydroperoxy intermediate¹⁵ that rapidly decomposes forming $\text{HOOCH}_2\text{SSCHO}$ and an OH radical. We calculated the rate coefficients of both H-shift reactions, $k_8 = 3.2 \times 10^{-2} \text{ s}^{-1}$ and $k_{10} = 3.3 \times 10^{-2} \text{ s}^{-1}$ at 298.15 K (see ESI). According to that, the isomerization steps (8) and (10) are competitive with RO_2 reactions with NO, HO_2 or other RO_2 radicals for pristine or moderately polluted conditions, similar to other,

atmospherically relevant RO_2 isomerization steps observed for functionalized hydrocarbons,¹⁸⁻²⁰ DMS ¹⁵⁻¹⁷ and amines.²¹

The importance of $\text{HOOCH}_2\text{SSCHO}$ formation for the whole product distribution of $\text{OH} + \text{DMDS}$ is small. The H-abstraction channel is expected to account only for about 2% of the overall $\text{OH} + \text{DMDS}$ reaction based on $k_{1a} + k_{1b} = 2.3 \times 10^{-10} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_{1b} = 4.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K²², the latter adopted from $\text{OH} + \text{DMS}$. In contrast, H-abstraction is the dominant path in the case of $\text{OH} + \text{DMS}$ at 295 - 299 K accounting for 65% of the DMS reaction.^{10, 16, 17} The relatively small signal intensities of $\text{O}_2\text{CH}_2\text{SSCH}_2\text{OOH}$ and $\text{HOOCH}_2\text{SSCHO}$ compared with the equivalent signals from the $\text{OH} + \text{DMS}$ reaction¹⁶ are in line with the minor importance of channel (1b).

SO_2 is the expected oxidation product of CH_3S for our conditions as well as in the atmosphere and is mainly formed via the reaction sequences (4),(5) and (6),(7),(5).^{10, 13} Sensitive SO_2 detection for concentrations down to $10^5 \text{ molecules cm}^{-3}$ has been achieved using SF_6^- and CO_3^- as the reagent ions: $\text{SF}_6^- + \text{SO}_2 \rightarrow \text{F}_2\text{SO}_2^- + \text{SF}_4$ ²³ and $\text{CO}_3^- + \text{SO}_2 (+\text{O}_2) \rightarrow \text{SO}_5^- + \text{CO}_2$ ²⁴, respectively. The very good agreement between the signal intensities arising from $^{32}\text{SO}_2$ and $^{34}\text{SO}_2$ according to their natural isotope abundance shows this approach also as a very selective method without distinct interference from other products (Fig.S3). SO_2 formation yields of 0.92 ± 0.19 (SF_6^-) and 0.89 ± 0.18 (CO_3^-) were obtained from $\text{OH} + \text{DMDS}$ for a low O_3 concentration of $1.6 \times 10^{10} \text{ molecules cm}^{-3}$ being in good agreement for both ionization schemes (Fig.S4). The stated error range includes 20 % uncertainty from absolute SO_2 calibration. For comparison, experiments on SO_2 formation from $\text{OH} + \text{CH}_3\text{SH}$ have been also conducted for otherwise identical reaction conditions.

A CH_3S formation yield of 1.1 ± 0.2 ²⁵ was reported from $\text{OH} + \text{CH}_3\text{SH}$ characterizing reaction (11) as a suitable CH_3S source. We measured a SO_2 formation yield of 0.86 ± 0.18 (SF_6^-) in good agreement with the SO_2 yield from $\text{OH} + \text{DMDS}$ for the same low O_3 conditions (Fig.S5). The agreement in both reaction systems suggests CH_3S as the important intermediate for SO_2 formation also in the $\text{OH} + \text{DMDS}$ reaction with an assumed CH_3S formation yield of close to unity. This would be in line with the expected main pathways (1a) and (2),^{1,9} but somewhat contrary to a CH_3S yield of 0.28 ± 0.20 from an earlier photolysis experiment.¹¹ The findings from our quantum chemical calculations show a fast dissociation reaction of $\text{CH}_3\text{SS}(\text{OH})\text{CH}_3$ into CH_3S and CH_3SOH from the addition channel via (1a) and (2), pointing to formation yields of close to unity for each (see ESI). Results from modelling confirmed the efficient SO_2 formation from CH_3S via reactions (3), (4) and (5) in air, even for our short residence time of 7.9 s, and the minor contribution of ozone reactions for $[\text{O}_3] = 1.6 \times 10^{10} \text{ molecules cm}^{-3}$ (see ESI).

Increasing O_3 concentrations led to further rise of the SO_2 yield from $\text{OH} + \text{DMDS}$ ending up at 2.18 ± 0.45 for $[\text{O}_3] = 1.3 \times 10^{12} \text{ molecules cm}^{-3}$ (Fig.1 and Table 1 showing the SO_2 yields). Atmospheric average ozone concentrations span a range of about $(5 - 10) \times 10^{11} \text{ molecules cm}^{-3}$, in most areas of the world. NO additions of up to $1.7 \times 10^{10} \text{ molecules cm}^{-3}$, representative

Scheme 1 First reaction steps of the atmospheric $\text{OH} + \text{DMDS}$ reaction. Known pathways from literature^{4-6, 10} are given in black and findings from this work in red. Minor reactions are indicated by dashed arrows and observed products by a frame. Possible $\text{CH}_3\text{SSCH}_2\text{O}_2$ reactions with NO, HO_2 or other RO_2 radicals are not shown.

Fig.1 SO₂ formation as a function of reacted DMDS for different O₃ concentrations. SO₂ detection via CO₃⁻ ionization. Error bars are omitted for more clarity. [DMDS] = 1.0 × 10¹¹ and [TME] = (1.0 - 160) × 10⁹ molecules cm⁻³.

for moderately polluted areas, resulted in only a small reduction of the SO₂ formation of ≤ 5% (Fig.S6).

The very high SO₂ yield, about twice the reacted DMDS, indicates that approximately both S atoms from the reactant are converted to SO₂ for high enough O₃ concentrations. That means, that also CH₃SOH has to form SO₂ (expecting again a CH₃SOH yield of close to unity from OH + DMDS). Atmospheric gas-phase reactions of CH₃SOH (methane sulfenic acid) are not reported so far including the envisaged reaction with O₃ relevant for our conditions.

Quantum chemical calculations suggest that CH₃SOH may react with O₃ in a concerted reaction via a transition state submerged by 4.2 kcal mol⁻¹ relative to the free reactants as shown in the energy diagram in Fig.2. For the formed intermediate CH₃S(O)OOH, there are two possible unimolecular decomposition channels; one occurring by a concerted reorganization and O₂-loss (grey in Fig.2) and the other by HO₂-loss (orange in Fig.2). The O₂-loss channel forms (CH₃S(O)OH (methane sulfinic acid) and singlet oxygen, the HO₂-loss channel CH₃S(O)O and HO₂. CH₃S(O)O will further react via reaction (5) forming SO₂ and CH₃. RRKM-ME simulations²⁶ showed that both unimolecular channels occur promptly via the excess energy from the O₃ + CH₃SOH reaction with a preference for the HO₂-loss channel by about 3:1 (see ESI). A rapid O₃ + CH₃SOH reaction with a preferred CH₃S(O)O production can explain the very high SO₂ yield of up to about twice of the reacted DMDS.

A weak signal consistent with the occurrence of CH₃S(O)OH from the O₂-loss channel was observed by applying iodide ionization. The signal linearly increased with rising DMDS conversion as expected from the formation kinetics of CH₃S(O)OH (Fig.S7). The lack of a reference substance prevented absolute signal calibration. A lower limit CH₃S(O)OH formation yield (assuming correct assignment) of 0.0091 ± 0.0003 has been obtained from measurements with [O₃] = 6.1 × 10¹¹ molecules cm⁻³. Despite the uncertainty in the CH₃S(O)OH determination, its formation seems to be less important for the substance balance of O₃ + CH₃SOH, in line with the findings from quantum chemical calculations.

Table 1. SO₂ formation yields from OH + DMDS (OH + CH₃SH) measured in air.

	O ₃ (molecules cm ⁻³)	SO ₂ yield ^a
OH + DMDS	1.6 × 10 ¹⁰	0.92 ± 0.19 ^b 0.89 ± 0.18 ^c
	3.2 × 10 ¹⁰	1.14 ± 0.23 ^c
	1.9 × 10 ¹¹	1.61 ± 0.35 ^c
	6.1 × 10 ¹¹	1.97 ± 0.48 ^c
	1.3 × 10 ¹²	2.18 ± 0.45 ^c
OH + CH ₃ SH	1.6 × 10 ¹⁰	0.86 ± 0.18 ^b

^a includes 20% uncertainty from SO₂ calibration. ^b SF₆⁻ ionization; ^c CO₃⁻ ionization

We experimentally tested also for the formation of methyl peroxy radicals CH₃O₂, promptly formed via CH₃ + O₂ in air, as the co-product of SO₂ from pathway (5). CH₃O₂ was indirectly followed via its accretion product ROOR arising from the RO₂ cross reaction with CH₃C(O)CH₂O₂, which is produced from TME ozonolysis as a by-product in the course of OH formation.²⁷

The CH₃C(O)CH₂OOCH₃ signal, measured by means of ethylammonium ionization, increased by a factor of about 4.5 when the RO₂ level in the experiment, CH₃C(O)CH₂O₂ and approximately also CH₃O₂, was increased by a factor of 2.2 (Fig.S8). This behaviour reflects the second-order kinetics of ROOR production via pathway (12). Quantitative information has been achieved by comparing the CH₃C(O)CH₂OOCH₃ signal intensity from OH + DMDS with that of OH + CH₄ using identical OH reactivities, i.e. k(OH+DMDS) × [DMDS] = k(OH+CH₄) × [CH₄].^{22, 28} A CH₃O₂ yield of unity is expected from the OH + CH₄ reaction. For [O₃] = 6.1 × 10¹¹ molecules cm⁻³ with an SO₂ yield of 1.97 ± 0.48 (Table 1), the DMDS reaction yielded a 1.4-times higher CH₃C(O)CH₂OOCH₃ signal than the CH₄ reaction pointing to a CH₃O₂ yield of at least 1.4 from OH + DMDS (Fig.S8). The reason for the lower bound assumption is the fact that CH₃O₂ production via OH + DMDS is delayed in time compared to the direct CH₃O₂ formation from OH + CH₄ mainly due to the intermediate O₃ + CH₃SOH reaction. The delay in CH₃O₂ production leads to less efficient ROOR formation via pathway (12) within the short residence time of 7.9 s. Nevertheless, a CH₃O₂ yield > 1.4 from OH + DMDS for [O₃] = 6.1 × 10¹¹ molecules cm⁻³ supports the high SO₂ yield of 1.97 ± 0.48.

Fig.2 Stationary points in the O₃-initiated CH₃SOH oxidation scheme calculated at the RO-CCSD(T)-F12a/VDZ-F12//ωB97X-D/aVTZ level. The reaction between CH₃SOH and ozone is shown in blue, the O₂-loss channel in grey and the HO₂-loss channel in orange. The molecular oxygen (O₂) is calculated at its singlet state.

Formation of MSA has been detected via the signal of its deprotonation product (MSA-H)⁻ measured by means of nitrate ionization and via the (MSA)I⁻ adduct using iodide ionization (Fig.S9). Results of both techniques consistently show a nearly quadratic signal increase with rising DMDS conversion. This behaviour points to a reaction of two intermediates from OH + DMDS forming finally MSA. The exact chemical nature of such a pathway is highly speculative at the moment. A maximum MSA formation yield of 0.0043 was obtained from nitrate ionization using absolute signal calibration for the structurally similar sulfuric acid (H₂SO₄). The much higher MSA yields of up to 0.14 observed in previous experiments were likely due to the much higher amounts of converted DMDS, potentially higher intermediate concentrations and the much longer reaction times applied.^{5,6}

We utilized biomass burning data from an emission inventory in order to examine the atmospheric relevance of the DMDS oxidation for the SO₂ budget.³ A DMDS contribution of 8 % to 54 % to the global biomass burning sulfur emission has been found based on available SO₂ and DMS emission data along with a DMDS/DMS ratio estimation (see ESI). Due to the rapid DMDS oxidation yielding two SO₂, the DMDS-derived SO₂ formation can be as high as the direct SO₂ emission demonstrating the importance of DMDS from biomass burning.

In conclusion, our combined experimental and theoretical results show that the atmospheric OH + CH₃SSCH₃ reaction mainly forms SO₂ and CH₃O₂ with a yield of both close to two. This process proceeds most likely via the OH-adduct CH₃S(OH)SCH₃ (addition channel) that rapidly decomposes forming CH₃S and CH₃SOH. CH₃S further reacts with O₂ and O₃, and CH₃SOH with O₃, both leading to CH₃S(O)O, which readily decomposes to SO₂ and CH₃. The subsequent CH₃ + O₂ reaction forms CH₃O₂. A minor path of O₃ + CH₃SOH results in CH₃S(O)OH. Product formation from O₃ + CH₃SOH is reported here for the first time. Observed products from the OH + CH₃SSCH₃ abstraction channel, that accounts for about 2 % of CH₃SSCH₃ conversion, are O₂CH₂SSCH₂OOH and HOOCH₂SSCHO formed via peroxy radical isomerization steps (Scheme 1).

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Conflicts of interest

There are no conflicts to declare.

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