

Table S6 Gas-phase reactions of DM1.0

Nr.	Reaction	k	-E _A /R [K]	Comment	Reference
gD1	CH ₃ SCH ₃ + OH → CH ₃ SCH ₂ (O ₂) - O ₂	1.12·10 ⁻¹¹	-250		(A)
gD2	CH ₃ SCH ₃ + OH → CH ₃ S(OH)CH ₃	(1)			(A)
gD3	CH ₃ S(OH)CH ₃ → CH ₃ SCH ₃ + OH	(2)			(E)
gD4	CH ₃ S(OH)CH ₃ + O ₂ → (CH ₃) ₂ S(OH)(O ₂)	8.50·10 ⁻¹³			(C)
gD5	CH ₃ S(OH)CH ₃ → CH ₃ S(OH) + CH ₃ (O ₂) - O ₂	5.00·10 ⁺⁰⁵			(D)
gD6	CH ₃ SCH ₃ + NO ₃ → CH ₃ SCH ₂ (O ₂) - O ₂	1.90·10 ⁻¹³	520		(A)
gD7	CH ₃ SCH ₃ + Cl → 0.45 CH ₃ SCH ₂ (O ₂) + 0.45 HCl + 0.55 (CH ₃) ₂ S(Cl) - 0.45 O ₂	3.40·10 ⁻¹⁰			(B)
gD8	CH ₃ SCH ₃ + Br → CH ₃ SCH ₂ (O ₂) + HBr - O ₂	9.00·10 ⁻¹¹	-2390		(C)
gD9	CH ₃ SCH ₃ + Br → (CH ₃) ₂ S(Br)	(3)			(C)
gD10	CH ₃ SCH ₃ + ClO → 0.73 Cl + 0.73 CH ₃ SOCH ₃ + 0.27 HOCl + 0.27 CH ₃ SCH ₂ (O ₂) - 0.27 O ₂	1.70·10 ⁻¹⁵	340		(B)
gD11	CH ₃ SCH ₃ + BrO → CH ₃ SOCH ₃ + Br	1.50·10 ⁻¹⁴	1000		(B)
gD12	CH ₃ SCH ₃ + Cl ₂ → CH ₃ SCH ₂ (Cl) + HCl	3.40·10 ⁻¹⁴			(F)
gD13	CH ₃ SCH ₃ + IO → CH ₃ SOCH ₃ + I	3.30·10 ⁻¹³	-925		(B)
gD14	CH ₃ SCH ₂ (O ₂) + HO ₂ → CH ₃ SCH ₂ (OOH) + O ₂	1.13·10 ⁻¹³	1300		(A)
gD15	CH ₃ SCH ₂ (O ₂) + NO → CH ₃ SCH ₂ (O) + NO ₂	4.90·10 ⁻¹²	260		(A)
gD16	CH ₃ SCH ₂ (O ₂) + NO ₃ → CH ₃ SCH ₂ (O) + NO ₂ + O ₂	2.30·10 ⁻¹²			(A)
gD17	CH ₃ SCH ₂ (O ₂) + RO ₂ → 0.8 CH ₃ SCH ₂ (O) + 0.1 CH ₃ SCH ₂ (OH) + 0.1 CH ₃ SCHO + O ₂	3.74·10 ⁻¹²			(A)
gD18	(CH ₃) ₂ S(OH)(O ₂) + NO → CH ₃ SO ₂ CH ₃ + HO ₂ + NO ₂ - O ₂	2.70·10 ⁻¹²	360		(A)
gD19	(CH ₃) ₂ S(OH)(O ₂) → CH ₃ SOCH ₃ + HO ₂	8.90·10 ⁺¹⁰	-6040		(A)
gD20	CH ₃ SCH ₂ (Cl) + OH → CH ₃ S(OH) + CH ₂ (Cl)(O ₂) - O ₂	2.50·10 ⁻¹²			(G)
gD21	(CH ₃) ₂ S(Cl) + NO ₂ → CH ₃ SCH ₃ + ClNO ₂	2.70·10 ⁻¹¹		products after ^(N)	(H)
gD22	(CH ₃) ₂ S(Cl) + NO → CH ₃ SCH ₃ + ClNO	1.20·10 ⁻¹¹		products after ^(N)	(H)
gD23	(CH ₃) ₂ S(Cl) + O ₂ → CH ₃ SOCH ₃ + ClO	4.00·10 ⁻¹⁸		(R)	(H)
gD24	(CH ₃) ₂ S(Cl) → CH ₃ SCH ₃ + Cl	9.00·10 ⁺⁰¹			(I)

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Nr.	Reaction	k	$-E_A/R$ [K]	Comment	Reference
gD25	$(\text{CH}_3)_2\text{S}(\text{Br}) + \text{O}_2 \rightarrow \text{CH}_3\text{SOCH}_3 + \text{BrO}$	$1.00 \cdot 10^{-18}$			(J)
gD26	$(\text{CH}_3)_2\text{S}(\text{Br}) \rightarrow \text{CH}_3\text{SCH}_3 + \text{Br}$	$1.02 \cdot 10^{+04}$			(J)
gD27	$\text{CH}_3\text{SCH}_2(\text{OOH}) + \text{OH} \rightarrow \text{CH}_3\text{SCHO} + \text{OH} + \text{H}_2\text{O}$	$7.03 \cdot 10^{-11}$			(A)
gD28	$\text{CH}_3\text{SCH}_2(\text{O}) \rightarrow \text{CH}_3\text{S} + \text{HCHO}$	$1.00 \cdot 10^{+06}$			(A)
gD29	$\text{CH}_3\text{SCH}_2(\text{OH}) + \text{OH} \rightarrow \text{CH}_3\text{SCHO} + \text{HO}_2 - \text{O}_2$	$2.78 \cdot 10^{-11}$			(A)
gD30	$\text{CH}_3\text{SCHO} + \text{OH} \rightarrow \text{CH}_3\text{S} + \text{CO} + \text{H}_2\text{O}$	$1.11 \cdot 10^{-11}$			(A)
gD31	$\text{CH}_3\text{SO}_2\text{CH}_3 + \text{OH} \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2(\text{O}_2) + \text{H}_2\text{O} - \text{O}_2$	$4.40 \cdot 10^{-14}$			(A)
gD32	$\text{CH}_3\text{SOCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{SO}_2\text{H} + \text{CH}_3(\text{O}_2) - \text{O}_2$	$6.10 \cdot 10^{-12}$	800		(A)
gD33	$\text{CH}_3\text{SOCH}_3 + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2\text{CH}_3 + \text{NO}_2$	$2.90 \cdot 10^{-13}$			(C)
gD34	$\text{CH}_3\text{SOCH}_3 + \text{Cl} \rightarrow \text{CH}_3\text{SOCH}_2(\text{O}_2) + \text{HCl} - \text{O}_2$	$1.45 \cdot 10^{-11}$			(K)
gD35	$\text{CH}_3\text{SOCH}_3 + \text{Cl} \rightarrow (\text{CH}_3)_2\text{SO}(\text{Cl})$	$7.40 \cdot 10^{-11}$			(L)
gD36	$\text{CH}_3\text{SOCH}_3 + \text{BrO} \rightarrow \text{CH}_3\text{SO}_2\text{CH}_3 + \text{Br}$	$1.00 \cdot 10^{-14}$			(M)
gD37	$(\text{CH}_3)_2\text{SO}(\text{Cl}) + \text{O}_2 \rightarrow \text{CH}_3\text{SO}_2\text{CH}_3 + \text{ClO}$	$3.00 \cdot 10^{-18}$		products after ^(N)	(N)
gD38	$(\text{CH}_3)_2\text{SO}(\text{Cl}) + \text{NO} \rightarrow \text{CH}_3\text{SOCH}_3 + \text{ClNO}$	$1.20 \cdot 10^{-11}$		products after ^(N)	(N)
gD39	$(\text{CH}_3)_2\text{SO}(\text{Cl}) + \text{NO}_2 \rightarrow \text{CH}_3\text{SOCH}_3 + \text{ClNO}_2$	$2.10 \cdot 10^{-11}$		products after ^(N)	(N)
gD40	$(\text{CH}_3)_2\text{SO}(\text{Cl}) + (\text{CH}_3)_2\text{SO}(\text{Cl}) \rightarrow 2 \text{CH}_3\text{SOCH}_3 + \text{Cl}_2$	$3.00 \cdot 10^{-11}$			(N)
gD41	$(\text{CH}_3)_2\text{SO}(\text{Cl}) \rightarrow \text{CH}_3\text{SOCH}_3 + \text{Cl}$	$9.00 \cdot 10^{+01}$		estimated as DMS	(I)
gD42	$\text{CH}_3\text{SOCH}_2(\text{O}_2) + \text{NO} \rightarrow \text{CH}_3\text{S}(\text{O}) + \text{HCHO} + \text{NO}_2$	$7.50 \cdot 10^{-12}$			(O)
gD43	$\text{CH}_3\text{SOCH}_2(\text{O}_2) + \text{HO}_2 \rightarrow \text{CH}_3\text{SOCH}_2(\text{OOH}) + \text{O}_2$	$1.50 \cdot 10^{-12}$			(D)
gD44	$\text{CH}_3\text{S}(\text{OH}) + \text{OH} \rightarrow \text{CH}_3\text{S}(\text{O}) + \text{H}_2\text{O}$	$5.00 \cdot 10^{-11}$			(E)
gD45	$\text{CH}_3\text{S} + \text{NO}_2 \rightarrow \text{CH}_3\text{S}(\text{O}) + \text{NO}$	$6.00 \cdot 10^{-11}$	240		(A)
gD46	$\text{CH}_3\text{S} + \text{O}_3 \rightarrow \text{CH}_3\text{S}(\text{O}) + \text{O}_2$	$1.15 \cdot 10^{-12}$	430		(A)
gD47	$\text{CH}_3\text{S} + \text{O}_2 \rightarrow \text{CH}_3\text{S}(\text{OO})$	$1.20 \cdot 10^{-16}$	1580		(A)
gD48	$\text{CH}_3\text{SO}_2\text{CH}_2(\text{O}_2) + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2(\text{OOH}) + \text{O}_2$	$1.13 \cdot 10^{-13}$	1300		(A)

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gD49	CH ₃ SO ₂ CH ₂ (O ₂) + NO → CH ₃ SO ₂ CH ₂ (O) + NO ₂	2.70·10 ⁻¹²	360		(A)
gD50	CH ₃ SO ₂ CH ₂ (O ₂) + NO ₃ → CH ₃ SO ₂ CH ₂ (O) + NO ₂ + O ₂	2.30·10 ⁻¹²			(A)
gD51	CH ₃ SO ₂ CH ₂ (O ₂) + RO ₂ → 0.2 CH ₃ SO ₂ CHO + 0.6 CH ₃ SO ₂ CH ₂ (O) + 0.2 CH ₃ SO ₂ CH ₂ (OH) + O ₂	2.00·10 ⁻¹²			(A)
gD52	CH ₃ SO ₂ H + OH → CH ₃ (O ₂) + SO ₂ + H ₂ O - O ₂	9.00·10 ⁻¹¹			(A)
gD53	CH ₃ SO ₂ H + NO ₃ → CH ₃ SO ₂ + HNO ₃	1.00·10 ⁻¹³			(D)
gD54	CH ₃ S(O) + NO ₂ → 0.25 CH ₃ (O ₂) + 0.25 SO ₂ + 0.25 NO - 0.25 O ₂ + 0.75 CH ₃ SO ₂ + 0.75 NO	1.20·10 ⁻¹¹			(A)
gD55	CH ₃ S(O) + O ₃ → CH ₃ (O ₂) + SO ₂	4.00·10 ⁻¹³			(A)
gD56	CH ₃ S(O) + O ₂ → CH ₃ S(O)(O ₂)	3.12·10 ⁻¹⁶	1580		(A)
gD57	CH ₃ S(OO) + HO ₂ → CH ₃ S(OOH) + O ₂	4.00·10 ⁻¹²			(D)
gD58	CH ₃ S(OO) + NO → CH ₃ S(O) + NO ₂	1.10·10 ⁻¹¹			(A)
gD59	CH ₃ S(OO) + NO ₂ → CH ₃ S(O) + NO ₃	2.20·10 ⁻¹¹			(A)
gD60	CH ₃ S(OO) → CH ₃ (O ₂) + SO ₂ - O ₂	5.60·10 ⁺¹⁶	-10870		(A)
gD61	CH ₃ S(OO) → CH ₃ S + O ₂	3.50·10 ⁺¹⁰	-3560		(A)
gD62	CH ₃ S(OO) → CH ₃ SO ₂	1.00·10 ⁰⁰		isomerisation after ^(P)	(S)
gD63	CH ₃ SO ₂ CH ₂ (OOH) + OH → CH ₃ SO ₂ CHO + OH + H ₂ O	1.26·10 ⁻¹²			(A)
gD64	CH ₃ SO ₂ CH ₂ (OOH) + OH → CH ₃ SO ₂ CH ₂ (O ₂) + H ₂ O	3.60·10 ⁻¹²			(A)
gD65	CH ₃ SO ₂ CH ₂ (O) → CH ₃ SO ₂ + HCHO	1.00·10 ⁺⁰⁶			(A)
gD66	CH ₃ SO ₂ CHO + OH → CH ₃ S(OO) + CO + H ₂ O	1.78·10 ⁻¹²			(A)
gD67	CH ₃ SO ₂ CH ₂ (OH) + OH → CH ₃ SO ₂ CHO + HO ₂ + H ₂ O - O ₂	5.23·10 ⁻¹³			(A)
gD68	CH ₃ SO ₂ CH ₂ (OH) + OH → CH ₃ SO ₂ CH ₂ (O) + H ₂ O	1.40·10 ⁻¹³			(A)
gD69	CH ₃ SO ₂ + OH → CH ₃ SO ₃ H	5.00·10 ⁻¹¹			(D)
gD70	CH ₃ SO ₂ + NO ₂ → CH ₃ SO ₃ + NO	2.20·10 ⁻¹¹			(C)
gD71	CH ₃ SO ₂ + O ₃ → CH ₃ SO ₃ + O ₂	3.00·10 ⁻¹³			(A)

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Nr.	Reaction	k	-E _A /R [K]	Comment	Reference
gD72	CH ₃ SO ₂ → CH ₃ (O ₂) + SO ₂ - O ₂	5.00·10 ⁺¹³	-9673		(A)
gD73	CH ₃ SO ₂ + O ₂ → CH ₃ SO ₂ (O ₂)	1.03·10 ⁻¹⁶	1580		(A)
gD74	CH ₃ SO(O ₂) + HO ₂ → 0.44 CH ₃ SO ₂ + 0.44 OH + 0.41 CH ₃ SO(OOH) + 0.15 CH ₃ SO ₂ H + 0.15 O ₃	5.20·10 ⁻¹³	980		(A)
gD75	CH ₃ SO(O ₂) + NO → CH ₃ SO ₂ + NO ₂	1.00·10 ⁻¹¹			(A)
gD76	CH ₃ SO(O ₂) + NO ₂ → CH ₃ SO ₃ NO ₂	(4)			(A)
gD77	CH ₃ SO(O ₂) + NO ₃ → CH ₃ SO ₂ + NO ₂ + O ₂	4.00·10 ⁻¹²			(A)
gD78	CH ₃ SO(O ₂) → CH ₃ SO + O ₂	9.10·10 ⁺¹⁰	-3560		(A)
gD79	CH ₃ SO(O ₂) + RO ₂ → 0.7 CH ₃ SO ₂ + 0.3 CH ₃ SO ₂ H + O ₂	1.00·10 ⁻¹¹			(A)
gD80	CH ₃ SO ₃ + HO ₂ → CH ₃ SO ₃ H + O ₂	5.00·10 ⁻¹¹			(A)
gD81	CH ₃ SO ₃ → CH ₃ O ₂ + SULF - H ₂ O - O ₂	5.00·10 ⁺¹³	-9946		(A)
gD82	CH ₃ SO ₂ (O ₂) + HO ₂ → 0.41 CH ₃ SO ₂ (OOH) + 0.44 CH ₃ SO ₃ + 0.44 OH + 0.15 CH ₃ SO ₃ H + 0.15 O ₃	5.20·10 ⁻¹³	980		(A)
gD83	CH ₃ SO ₂ (O ₂) + NO → CH ₃ SO ₃ + NO ₂	1.00·10 ⁻¹¹			(A)
gD84	CH ₃ SO ₂ (O ₂) + NO ₂ → CH ₃ SO ₄ NO ₂	(4)			(A)
gD85	CH ₃ SO ₂ (O ₂) + NO ₃ → CH ₃ SO ₃ + NO ₂ + O ₂	4.00·10 ⁻¹²			(A)
gD86	CH ₃ SO ₂ (O ₂) → CH ₃ SO ₂ + O ₂	3.01·10 ⁺¹⁰	-3560		(A)
gD87	CH ₃ SO ₂ (O ₂) + RO ₂ → 0.7 CH ₃ SO ₃ + 0.3 CH ₃ SO ₃ H + O ₂	1.00·10 ⁻¹¹			(A)
gD88	CH ₃ SO(OOH) + OH → CH ₃ SO(O ₂) + H ₂ O	9.00·10 ⁻¹¹			(A)
gD89	CH ₃ SO ₃ NO ₂ + OH → CH ₃ SO ₂ H + NO ₂ + O ₂	1.00·10 ⁻¹¹			(A)
gD90	CH ₃ SO ₃ NO ₂ → CH ₃ SO(O ₂) + NO ₂	5.40·10 ⁺¹⁶	-13112		(A)
gD91	CH ₃ SO ₃ H + OH → CH ₃ SO ₃ + H ₂ O	2.24·10 ⁻¹⁴			(A)
gD92	CH ₃ SO ₂ (OOH) + OH → CH ₃ SO ₂ (O ₂) + H ₂ O	3.60·10 ⁻¹²			(A)
gD93	CH ₃ SO ₄ NO ₂ + OH → CH ₃ SO ₂ (O ₂) + HNO ₃	3.60·10 ⁻¹³			(A)

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Nr.	Reaction	k	-E _A /R [K]	Comment	Reference
gD94	CH ₃ SO ₄ NO ₂ → CH ₃ SO ₂ (O ₂) + NO ₂	5.40·10 ⁺¹⁶³	-13112		(A)

$$k_1: 9.5 \cdot 10^{-39} \cdot \text{O}_2 \cdot \exp(5270/\text{TEMP}) / (1 + 7.5 \cdot 10^{-29} \cdot \text{O}_2 \cdot \exp(5610/\text{TEMP}))$$

$$k_2 = k_1 / K_{\text{eq}} \text{ mit } k_1: 1.7 \cdot 10^{-42} \cdot \text{O}_2 \cdot \exp(7810/\text{TEMP}) / (1 + 5.5 \cdot 10^{-31} \cdot \text{O}_2 \cdot \exp(7460/\text{TEMP})) \text{ und } K_{\text{eq}}: 8.3 \cdot 10^{-29} \cdot \text{TEMP} \cdot \exp(5136/\text{TEMP})$$

$$K_3: 3.7 \cdot 10^{-29} \cdot (\text{TEMP}/300)^{-5.3} \text{ (low pressure)} \quad 1.5 \cdot 10^{-10} \cdot (\text{TEMP}/300)^{-2} \text{ (high pressure)}$$

$$K_4: 1.20 \cdot 10^{-12} \cdot (\text{TEMP}/300)^{-0.9}$$

(A) MCMv3.2, (B) IUPAC, (C) Sander et al. (7), (D) Yin et al. (60), (E) Lucas and Prinn (9), (F) Dyke et al. (61), (G) Shallcross et al. (62), (H) Urbanski and Wine (63), (I) Enami et al. (64), (J) Nakano et al. (65), (K) Nicovich et al. (66), (L) Falbe-Hansen et al. (67), (M) Ballesteros et al. (68), (N) Kleissas et al. (69), (O) Copeland et al. (70), (P) Turnipseed et al. (10), (R) Barnes et al. (8), (S) Campolongo et al. (11)

Table S7 Gas-phase photolysis of DM1.0

Nr	Reaction	I [s ⁻¹]	M	N	Reference
gPD01	CH ₃ SCH ₂ (OOH) → CH ₃ SCH ₂ (O) + OH	7.649·10 ⁻⁰⁶	0.682	0.279	MCMv3.2
gPD02	CH ₃ SCHO → CH ₃ S + CO + HO ₂ - O ₂	2.792·10 ⁻⁰⁵	0.805	0.338	MCMv3.2
gPD03	CH ₃ SO ₂ CH ₂ (OOH) → CH ₃ SO ₂ CH ₂ (O) + OH	7.649·10 ⁻⁰⁶	0.682	0.279	MCMv3.2
gPD04	CH ₃ SO ₂ CHO → CH ₃ SO ₂ + CO + HO ₂ - O ₂	2.792·10 ⁻⁰⁵	0.805	0.338	MCMv3.2
gPD05	CH ₃ SO(OOH) → CH ₃ SO ₂ + OH	7.649·10 ⁻⁰⁶	0.682	0.279	MCMv3.2
gPD06	CH ₃ SO ₂ (OOH) → CH ₃ SO ₃ + OH	7.649·10 ⁻⁰⁶	0.682	0.279	MCMv3.2
gPD07	CH ₃ SOCH ₂ (OOH) → CH ₃ S(O) + HCHO + OH	7.649·10 ⁻⁰⁶	0.682	0.279	Copeland et al. (70)
gPD08	CH ₃ SCH ₂ (Cl) → CH ₃ S + (Cl)CH ₂ (O ₂) - O ₂	1.458·10 ⁻⁰⁴	0.314	0.641	Copeland et al. (70)
gPD09	CH ₃ S(OOH) → CH ₃ S(O) + OH	7.649·10 ⁻⁰⁶	0.682	0.279	estimated as CH ₃ SCH ₂ OOH

Photolysis reactions are parameterized with $j_i = I \cdot \cos^{M_i} \cdot \exp(-N_i \cdot \sec \chi)$ (χ is the solar zenith angle) for more details see MCM (<http://mcm.leeds.ac.uk/MCMv3.1/>.)

Table S8 Phase transfer data of DM1.0

Species	$K_{H, 298}$, [M atm ⁻¹]	$-\Delta H/R$, [K]	Reference	α	Reference	D_g (298 K) [m ² s ⁻¹]	Reference
CH ₃ SCH ₃	0.56	4480	Campolongo et al. (11)	0.001	Zhu et al. (13)	$1.08 \cdot 10^{-5}$	Fuller et al. (16)
CH ₃ SOCH ₃	$1.00 \cdot 10^7$	2580	Campolongo et al. (11)	0.1	De Bruyn et al. (15)	$1.01 \cdot 10^{-5}$	Fuller et al. (16)
CH ₃ SO ₂ CH ₃	$1.00 \cdot 10^7$	5390	Campolongo et al. (11)	0.1	De Bruyn et al. (15)	$9.55 \cdot 10^{-6}$	Fuller et al. (16)
CH ₃ SO ₂ H	$1.00 \cdot 10^8$	1760	after Barnes et al. (8) and Campolongo et al. (11)	0.1	as MSA	$1.11 \cdot 10^{-5}$	Fuller et al. (16)
CH ₃ SO ₃ H	$1.00 \cdot 10^9$	1760	Campolongo et al. (11)	0.1	De Bruyn et al. (15)	$1.04 \cdot 10^{-5}$	Fuller et al. (16)

Table S9 Aqueous-phase reactions of DM1.0

Nr.	Reaction	k_{298}	$-E_A/R$	Comment	Reference
aD1	CH ₃ SCH ₃ + O ₃ → CH ₃ SOCH ₃ + O ₂	$8.61 \cdot 10^{+08}$	-2600		(AA)
aD2	CH ₃ SCH ₃ + OH → CH ₃ SOCH ₃ + HO ₂ - O ₂	$1.90 \cdot 10^{+10}$			(AB)
aD3	CH ₃ SCH ₃ + Cl ₂ ⁻ → (CH ₃) ₂ S(Cl) + Cl ⁻	$3.00 \cdot 10^{+09}$			(AC)
aD4	CH ₃ SCH ₃ + Br ₂ ⁻ → (CH ₃) ₂ S(Br) + Br ⁻	$3.20 \cdot 10^{+09}$			(AC)
aD5	CH ₃ SCH ₃ + H ₂ O ₂ → CH ₃ SOCH ₃ + H ₂ O	$3.40 \cdot 10^{+02}$			(AD)
aD6	(CH ₃) ₂ S(Cl) + O ₂ → CH ₃ SOCH ₃ + ClO	$2.41 \cdot 10^{+03}$		estimated out of gas phase	(AU)
aD7	(CH ₃) ₂ S(Br) + O ₂ → CH ₃ SOCH ₃ + BrO	$6.02 \cdot 10^{+02}$		estimated out of gas phase	(AV)
aD8	CH ₃ SOCH ₃ + O ₃ → CH ₃ SO ₂ CH ₃ + O ₂	$7.00 \cdot 10^{+00}$			(AE)
aD9	CH ₃ SOCH ₃ + OH → CH ₃ SO ₂ H + CH ₃	$6.65 \cdot 10^{+09}$	-1270		(AF)
aD10	CH ₃ SOCH ₃ + SO ₄ ⁻ → CH ₃ SOCH ₃ ⁺ + SO ₄ ²⁻	$2.97 \cdot 10^{+09}$	-1440		(AG)
aD11	CH ₃ SOCH ₃ + Cl → (CH ₃) ₂ SO(Cl)	$6.30 \cdot 10^{+09}$			(AH)
aD12	CH ₃ SOCH ₃ + Cl ₂ ⁻ → (CH ₃) ₂ SO(Cl) + Cl ⁻	$1.60 \cdot 10^{+07}$			(AH)
aD13	CH ₃ SOCH ₃ + H ₂ O ₂ → CH ₃ SO ₂ CH ₃ + H ₂ O	$2.75 \cdot 10^{+06}$			(AI)
aD14	CH ₃ SOCH ₃ ⁺ + Br ⁻ → (CH ₃) ₂ SO(Br)	$5.00 \cdot 10^{+09}$		measured in DMSO solution	(AJ)
aD15	(CH ₃) ₂ SO(Br) + Br ⁻ → CH ₃ SOCH ₃ + Br ₂ ⁻	$2.60 \cdot 10^{+08}$		measured in DMSO solution	(AJ)

Table S9 Aqueous-phase reactions of DM1.0

Nr.	Reaction	k_{298}	$-E_A/R$	Comment	Reference
aD16	$(\text{CH}_3)_2\text{SO}(\text{Cl}) + \text{H}_2\text{O} \rightarrow \text{CH}_3\text{SO}_2\text{H} + \text{HCl} + \text{CH}_3$	$1.00 \cdot 10^{+07}$			after ^(AK)
aD17	$(\text{CH}_3)_2\text{SO}(\text{OH}) \rightarrow \text{CH}_3\text{SO}_2\text{H} + \text{CH}_3$	$1.00 \cdot 10^{+07}$			(AL)
aD18	$\text{CH}_3\text{SO}_2\text{CH}_3 + \text{OH} \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2 + \text{H}_2\text{O}$	$1.77 \cdot 10^{+07}$	-1690	H-abstraction assumed	(AF)
aD19	$\text{CH}_3\text{SO}_2\text{CH}_3 + \text{SO}_4^- \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2 + \text{SO}_4^{2-} + \text{H}^+$	$3.95 \cdot 10^{+06}$	-1360	H-abstraction assumed	(AG)
aD20	$\text{CH}_3\text{SO}_2\text{CH}_3 + \text{Cl} \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2 + \text{HCl}$	$8.20 \cdot 10^{+05}$		H-abstraction assumed	(AH)
aD21	$\text{CH}_3\text{SO}_2\text{CH}_3 + \text{Cl}_2^- \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2 + \text{HCl} + \text{Cl}^-$	$8.24 \cdot 10^{+03}$		H-abstraction assumed	(AH)
aD22	$\text{CH}_3\text{SO}_2\text{CH}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{SO}_2\text{CH}_2(\text{O}_2)$	$2.00 \cdot 10^{+09}$			k estimated after ^(AM)
aD23	$\text{CH}_3\text{SO}_2\text{CH}_2(\text{O}_2) + \text{RO}_2 \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO} + \text{O}_2$	$7.00 \cdot 10^{+03}$			k estimated same as $(\text{O}_2)\text{CH}(\text{OH})(\text{SO}_3^-)$
aD24	$\text{CH}_3\text{SO}_2\text{H} + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3\text{H} + \text{O}_2$	$3.50 \cdot 10^{+07}$			(AE)
aD25	$\text{CH}_3\text{SO}_2\text{H} + \text{OH} \rightarrow \text{CH}_3\text{SO}(\text{OH})(\text{OH})$	$6.00 \cdot 10^{+09}$			(AE)
aD26	$\text{CH}_3\text{SO}_2^- + \text{OH} \rightarrow 0.9 \text{CH}_3\text{SO}_2 + 0.9 \text{OH}^- + 0.1 \text{CH}_3 + 0.1 \text{HSO}_3^-$	$1.20 \cdot 10^{+10}$		products after ^(AQ)	(AN)
aD27	$\text{CH}_3\text{SO}_2^- + \text{SO}_4^- \rightarrow \text{CH}_3\text{SO}_2 + \text{SO}_4^{2-}$	$1.00 \cdot 10^{+09}$		products after ^(AQ)	(AO)
aD28	$\text{CH}_3\text{SO}_2^- + \text{Cl}_2^- \rightarrow \text{CH}_3\text{SO}_2 + 2 \text{Cl}^-$	$8.00 \cdot 10^{+08}$		ETR assumed	(AK)
aD29	$\text{CH}_3\text{SO}_2^- + \text{H}_2\text{O}_2 \rightarrow \text{CH}_3\text{SO}_3^- + \text{H}_2\text{O}$	$1.20 \cdot 10^{+02}$			(AN)
aD30	$\text{CH}_3\text{SO}_2^- + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3^- + \text{O}_2$	$2.00 \cdot 10^{+06}$			(AQ)
aD31	$\text{CH}_3\text{SO}(\text{OH})(\text{OH}) + \text{O}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H} + \text{HO}_2$	$1.20 \cdot 10^{+09}$			(AE)
aD32	$\text{CH}_3\text{SO}_3\text{H} + \text{OH} \rightarrow \text{CH}_2\text{SO}_3\text{H} + \text{H}_2\text{O}$	$1.50 \cdot 10^{+07}$			(AE)
aD33	$\text{CH}_3\text{SO}_3^- + \text{OH} \rightarrow \text{CH}_2\text{SO}_3^- + \text{H}_2\text{O}$	$1.29 \cdot 10^{+07}$	-2630	H-abstraction assumed	(AF)
aD34	$\text{CH}_3\text{SO}_3^- + \text{SO}_4^- \rightarrow \text{CH}_3\text{SO}_3 + \text{SO}_4^{2-}$	$1.13 \cdot 10^{+04}$	-2490	ETR assumed	(AG)
aD35	$\text{CH}_3\text{SO}_3^- + \text{Cl} \rightarrow \text{CH}_3\text{SO}_3 + \text{Cl}^-$	$4.90 \cdot 10^{+05}$		ETR assumed	(AH)
aD36	$\text{CH}_3\text{SO}_3^- + \text{Cl}_2^- \rightarrow \text{CH}_3\text{SO}_3 + 2 \text{Cl}^-$	$3.89 \cdot 10^{+03}$		ETR assumed	(AH)
aD37	$\text{CH}_3\text{SO}_2 + \text{OH} \rightarrow \text{CH}_3\text{SO}_3\text{H}$	$1.00 \cdot 10^{+10}$		k estimated as $\text{CH}_3\text{SO}_2\text{H}$	
aD38	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3 + \text{O}_2$	$1.50 \cdot 10^{+09}$		k estimated as CH_2COO^-	(AP)

Table S9 Aqueous-phase reactions of DM1.0

Nr.	Reaction	k_{298}	$-E_A/R$	Comment	Reference
aD39	$\text{CH}_3\text{SO}_2 + \text{SO}_3^{2-} \rightarrow \text{CH}_3\text{SO}_2^- + \text{SO}_4^{2-} + 2 \text{H}^+ - \text{H}_2\text{O}$	$1.70 \cdot 10^{+09}$			(AQ)
aD40	$\text{CH}_3\text{SO}_2 \rightarrow \text{CH}_3 + \text{SO}_2$	$8.30 \cdot 10^{+04}$		in CH_3CN solution	(AR)
aD41	$\text{CH}_3\text{SO}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{SO}_2(\text{O}_2)$	$1.20 \cdot 10^{+09}$			(AS)
aD42	$2 \text{CH}_3\text{SO}_2 \rightarrow \text{CH}_3\text{SO}_2\text{H} + \text{CH}_3\text{SO}_3\text{H} - \text{H}_2\text{O}$	$9.00 \cdot 10^{+08}$			(AQ)
aD43	$\text{CH}_3\text{SO}_2(\text{O}_2) + \text{CH}_3\text{SO}_2^- \rightarrow \text{CH}_3\text{SO}_3^- + \text{CH}_3\text{SO}_3$	$6.20 \cdot 10^{+08}$			(AQ)
aD44	$\text{CH}_3\text{SO}_3 + \text{CH}_3\text{SO}_2^- \rightarrow \text{CH}_3\text{SO}_3^- + \text{CH}_3\text{SO}_2$	$1.00 \cdot 10^{+08}$			(AT)
aD45	$\text{CH}_3\text{SO}_3 \rightarrow \text{CH}_3 + \text{SO}_3$	$8.30 \cdot 10^{+04}$		estimated ($k_{\text{aD44}} \approx k_{\text{aD39}}$)	(AR)
aD46	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H} + \text{O}_2$	$8.30 \cdot 10^{+05}$			k estimated same as HO_2 recombination in CAPRAM
aD47	$\text{CH}_2\text{SO}_3\text{H} + \text{O}_2 \rightarrow (\text{O}_2)\text{CH}_2\text{SO}_3\text{H}$	$2.00 \cdot 10^{+09}$			k estimated after ^(AM)
aD48	$\text{CH}_2\text{SO}_3^- + \text{O}_2 \rightarrow (\text{O}_2)\text{CH}_2\text{SO}_3^-$	$2.00 \cdot 10^{+09}$			k estimated after ^(AM)
aD49	$2 ((\text{O}_2)\text{CH}_2\text{SO}_3^- + \text{H}^+) \rightarrow 2 \text{HCHO} + 2 \text{H}^+ + 2 \text{SO}_3^- + \text{O}_2$	$7.00 \cdot 10^{+03}$		reaction scheme after ^(AT)	k estimated same as $(\text{O}_2)\text{CH}(\text{OH})(\text{SO}_3^-)$

(AA) Gershenson et al. (24), (AB) Bonifacic et al. (71), (AC) Bonifacic and Asmus (21), (AD) Adewuyi and Carmichael (72), (AE) Herrmann and Zellner (17), (AF) Zhu et al. (73), (AG) Zhu et al. (74), (AH) Zhu (75), (AI) Amels et al. (76), (AJ) Sumiyoshi et al. (77), (AK) Zhu et al. (78), (AL) Kishore and Asmus (79), (AM) von Sonntag (80), (AN) Bardouki et al. (81), (AO) Zhu et al. (13), (AP) Sehested et al. (82), (AQ) Flyunt et al. (19), (AR) Robert-Banchereau et al. (83), (AS) Sehested and Holcman (84), (AT) Lee et al. (85), (AU) Urbanski and Wine (63), (AV) Nakano et al. (65)

Table S10 Aqueous-phase equilibriums of DM1.0

Equilibrium	K	E/R	$k_{298,\text{forward}}$	$k_{298,\text{(back)}}$	Reference
$\text{CH}_3\text{SO}_2\text{H} \rightleftharpoons \text{CH}_3\text{SO}_2^- + \text{H}^+$	$5.0 \cdot 10^{-03}$		$2.50 \cdot 10^{08}$	$5.00 \cdot 10^{10}$	Wudl et al. (86)
$\text{CH}_3\text{SO}_3\text{H} \rightleftharpoons \text{CH}_3\text{SO}_3^- + \text{H}^+$	73		$3.65 \cdot 10^{12}$	$5.00 \cdot 10^{10}$	Clarke and Woodward (87)
$(\text{O}_2)\text{CH}_2\text{SO}_3\text{H} \rightleftharpoons (\text{O}_2)\text{CH}_2\text{SO}_3^- + \text{H}^+$	73		$3.65 \cdot 10^{12}$	$5.00 \cdot 10^{10}$	estimated as $\text{CH}_3\text{SO}_3\text{H}$
$\text{Cl}^- + \text{CH}_3\text{SOCH}_3^+ \rightleftharpoons (\text{CH}_3)_2\text{SO}(\text{Cl})$	330		$1.00 \cdot 10^{10}$	$3.03 \cdot 10^{07}$	Zhu et al. (78)
$\text{CH}_3\text{SOCH}_3^+ + \text{H}_2\text{O} \rightleftharpoons (\text{CH}_3)_2\text{SO}(\text{OH}) + \text{H}^+$	$2.5 \cdot 10^{-06}$		$1.25 \cdot 10^{05}$	$5.00 \cdot 10^{10}$	Kishore and Asmus (79)

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