

The Chemical Mechanism of MECCA

KPP version: 2.2.3_rs3

MECCA version: 3.8t

Date: June 29, 2018

Batch file: simple_MADE.bat

Replacement file: mim1-simple_MADE

Selected reactions:

“Tr && G && (S | | !C) && !Cl && !Br && !I && !Hg”

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase: 34

Aqueous phase: 0

All species: 34

Number of reactions in selected mechanism:

Gas phase (Gnn): 47

Aqueous phase (Annn): 0

Henry (Hnn): 0

Photolysis (Jnn): 13

Aqueous phase photolysis (PHnn): 0

Heterogeneous (HETnn): 0

Equilibria (EQnn): 0

Isotope exchange (IEXnn): 0

Tagging equations (TAGnn): 0

Dummy (Dnn): 0

All equations: 60

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	UpStTrG	$\text{O}_2 + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{O}_2$	$3.3\text{E}-11 \cdot \text{EXP}(55./\text{temp})$	Burkholder et al. (2015)
G1001	UpStTrG	$\text{O}_2 + \text{O}(^3\text{P}) \rightarrow \text{O}_3$	$6.0\text{E}-34 \cdot ((\text{temp}/300.)^{**}(-2.4))$ *cair	Burkholder et al. (2015)
G2100	UpStTrG	$\text{H} + \text{O}_2 \rightarrow \text{HO}_2$	$\text{k_3rd}(\text{temp}, \text{cair}, 4.4\text{E}-32, 1.3,$ $7.5\text{E}-11, -0.2, 0.6)$	Burkholder et al. (2015)
G2104	UpStTrG	$\text{OH} + \text{O}_3 \rightarrow \text{HO}_2 + \text{O}_2$	$1.7\text{E}-12 \cdot \text{EXP}(-940./\text{temp})$	Burkholder et al. (2015)
G2105	UpStTrG	$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$	$2.8\text{E}-12 \cdot \text{EXP}(-1800./\text{temp})$	Burkholder et al. (2015)
G2107	UpStTrG	$\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + 2 \text{O}_2$	$1.\text{E}-14 \cdot \text{EXP}(-490./\text{temp})$	Burkholder et al. (2015)
G2109	UpStTrG	$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}_2$	$4.8\text{E}-11 \cdot \text{EXP}(250./\text{temp})$	Burkholder et al. (2015)
G2110	UpStTrG	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	k_HO2_HO2	Burkholder et al. (2015)*
G2111	UpStTrG	$\text{H}_2\text{O} + \text{O}(^1\text{D}) \rightarrow 2 \text{OH}$	$1.63\text{E}-10 \cdot \text{EXP}(60./\text{temp})$	Burkholder et al. (2015)
G2112	UpStTrG	$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HO}_2$	$1.8\text{E}-12$	Burkholder et al. (2015)
G2117	UpStTrG	$\text{H}_2\text{O} + \text{H}_2\text{O} \rightarrow (\text{H}_2\text{O})_2$	$6.521\text{E}-26 \cdot \text{temp} \cdot \text{EXP}(1851.09/\text{temp})$ * $\text{EXP}(-5.10485\text{E}-3 \cdot \text{temp})$	Scribano et al. (2006)*
G2118	UpStTrG	$(\text{H}_2\text{O})_2 \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}$	1.E0	see note*
G3101	UpStTrGN	$\text{N}_2 + \text{O}(^1\text{D}) \rightarrow \text{O}(^3\text{P}) + \text{N}_2$	$2.15\text{E}-11 \cdot \text{EXP}(110./\text{temp})$	Burkholder et al. (2015)
G3103	UpStTrGN	$\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$	$3.0\text{E}-12 \cdot \text{EXP}(-1500./\text{temp})$	Burkholder et al. (2015)
G3106	StTrGN	$\text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2$	$1.2\text{E}-13 \cdot \text{EXP}(-2450./\text{temp})$	Burkholder et al. (2015)
G3108	StTrGN	$\text{NO}_3 + \text{NO} \rightarrow 2 \text{NO}_2$	$1.5\text{E}-11 \cdot \text{EXP}(170./\text{temp})$	Burkholder et al. (2015)
G3109	UpStTrGN	$\text{NO}_3 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_5$	k_N03_NO2	Burkholder et al. (2015)*
G3110	StTrGN	$\text{N}_2\text{O}_5 \rightarrow \text{NO}_2 + \text{NO}_3$	$\text{k_N03_NO2}/(5.8\text{E}-27 \cdot \text{EXP}(10840./$ $\text{temp}))$	Burkholder et al. (2015)*
G3200	TrGN	$\text{NO} + \text{OH} \rightarrow \text{HONO}$	$\text{k_3rd}(\text{temp}, \text{cair}, 7.0\text{E}-31, 2.6,$ $3.6\text{E}-11, 0.1, 0.6)$	Burkholder et al. (2015)
G3201	UpStTrGN	$\text{NO} + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH}$	$3.3\text{E}-12 \cdot \text{EXP}(270./\text{temp})$	Burkholder et al. (2015)
G3202	UpStTrGN	$\text{NO}_2 + \text{OH} \rightarrow \text{HNO}_3$	$\text{k_3rd}(\text{temp}, \text{cair}, 1.8\text{E}-30, 3.0,$ $2.8\text{E}-11, 0., 0.6)$	Burkholder et al. (2015)
G3203	StTrGN	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	k_N02_HO2	Burkholder et al. (2015)*
G3204	TrGN	$\text{NO}_3 + \text{HO}_2 \rightarrow \text{NO}_2 + \text{OH} + \text{O}_2$	$3.5\text{E}-12$	Burkholder et al. (2015)
G3205	TrGN	$\text{HONO} + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.8\text{E}-11 \cdot \text{EXP}(-390./\text{temp})$	Burkholder et al. (2015)
G3206	StTrGN	$\text{HNO}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + \text{NO}_3$	k_HNO3_OH	Dulitz et al. (2018)*
G3207	StTrGN	$\text{HNO}_4 \rightarrow \text{NO}_2 + \text{HO}_2$	$\text{k_N02_HO2}/(2.1\text{E}-27 \cdot \text{EXP}(10900./$ $\text{temp}))$	Burkholder et al. (2015)*
G3208	StTrGN	$\text{HNO}_4 + \text{OH} \rightarrow \text{NO}_2 + \text{H}_2\text{O}$	$1.3\text{E}-12 \cdot \text{EXP}(380./\text{temp})$	Burkholder et al. (2015)

Table 1: Gas phase reactions (... continued)

#	labels	reaction	rate coefficient	reference
G4101	StTrG	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$	$1.85\text{E}-20 \cdot \text{EXP}(2.82 \cdot \text{LOG}(\text{temp}) - 987./\text{temp})$	Atkinson (2003)
G4102	TrG	$\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{HCHO} + \text{HO}_2$	$2.9\text{E}-12 \cdot \text{EXP}(-345./\text{temp})$	Sander et al. (2011)
G4103	StTrG	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	$4.1\text{E}-13 \cdot \text{EXP}(750./\text{temp})$	Sander et al. (2011)*
G4104	UpStTrGN	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.8\text{E}-12 \cdot \text{EXP}(300./\text{temp})$	Sander et al. (2011)
G4105	TrGN	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$	$1.3\text{E}-12$	Atkinson et al. (2006)
G4106a	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2 \text{HCHO} + 2 \text{HO}_2$	$9.5\text{E}-14 \cdot \text{EXP}(390./\text{temp}) / (1. + 26.2 \cdot \text{EXP}(1130./\text{temp}))$	Sander et al. (2011)
G4106b	StTrG	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH} + \text{O}_2$	$9.5\text{E}-14 \cdot \text{EXP}(390./\text{temp}) / (1. + 26.2 \cdot \text{EXP}(-1130./\text{temp}))$	Sander et al. (2011)
G4107	StTrG	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{CH}_3\text{O}_2 + .3 \text{HCHO} + .3 \text{OH} + \text{H}_2\text{O}$	$k_{\text{CH3OOH_OH}}$	Wallington et al. (2017)
G4108	StTrG	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E}-18 \cdot \text{EXP}(2.03 \cdot \text{LOG}(\text{temp}) + 636./\text{temp})$	Sivakumaran et al. (2003)
G4109	TrGN	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E}-13 \cdot \text{EXP}(-1900./\text{temp})$	Sander et al. (2011)*
G4110	UpStTrG	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$(1.57\text{E}-13 + \text{cair} \cdot 3.54\text{E}-33)$	McCabe et al. (2001)
G4111	TrG	$\text{HCOOH} + \text{OH} \rightarrow \text{CO}_2 + \text{HO}_2 + \text{H}_2\text{O}$	$4.0\text{E}-13$	Sander et al. (2011)
G9200	StTrGS	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	$k_{\text{3rd}}(\text{temp}, \text{cair}, 3.3\text{E}-31, 4.3, 1.6\text{E}-12, 0., 0.6)$	Burkholder et al. (2015)
G9400a	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E}-11 \cdot \text{EXP}(-253./\text{temp})$	Atkinson et al. (2004)*
G9400b	TrGCS	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	$k_{\text{DMS_OH}}$	Atkinson et al. (2004)*
G9401	TrGCNS	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E}-13 \cdot \text{EXP}(520./\text{temp})$	Atkinson et al. (2004)
G9402	TrGCS	$\text{DMSO} + \text{OH} \rightarrow .6 \text{SO}_2 + \text{HCHO} + .6 \text{CH}_3\text{O}_2 + .4 \text{HO}_2 + .4 \text{CH}_3\text{SO}_3\text{H}$	$1\text{E}-10$	Hynes and Wine (1996)
G9403	TrGS	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3\text{O}_2$	$1.8\text{E}13 \cdot \text{EXP}(-8661./\text{temp})$	Barone et al. (1995)
G9404	TrGS	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	$3\text{E}-13$	Barone et al. (1995)
G9405	TrGS	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	$5\text{E}-11$	Barone et al. (1995)

General notes

Three-body reactions

Rate coefficients for three-body reactions are defined via the function `k_3rd`($T, M, k_0^{300}, n, k_{\text{inf}}^{300}, m, f_c$). In the code, the temperature T is called `temp` and the concentration of “air molecules” M is called `cair`. Using the auxiliary variables $k_0(T)$, $k_{\text{inf}}(T)$, and k_{ratio} , `k_3rd` is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \quad (1)$$

$$k_{\text{inf}}(T) = k_{\text{inf}}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \quad (2)$$

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (3)$$

$$\text{k_3rd} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c^{\left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}})/N)^2}\right)} \quad (4)$$

A similar function, called `k_3rd_iupac` here, is used by Wallington et al. (2017) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \quad (5)$$

$$k_{\text{inf}}(T) = k_{\text{inf}}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \quad (6)$$

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (7)$$

$$N = 0.75 - 1.27 \times \log_{10}(f_c) \quad (8)$$

$$\text{k_3rd_iupac} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c^{\left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}})/N)^2}\right)} \quad (9)$$

RO₂ self and cross reactions

The self and cross reactions of organic peroxy radicals are treated according to the permutation reaction formalism as implemented in the MCM (Rickard and Pascoe, 2009), as described by Jenkin et al. (1997). Every organic peroxy radical reacts in a pseudo-first-order reaction with a rate constant that is expressed as $k^{\text{1st}} = 2 \times \sqrt{k_{\text{self}}} \times \text{k_CH3O2} \times [\text{RO}_2]$ where k_{self} = second-order rate coefficient of the self reaction of the organic peroxy radical, `k_CH3O2` = second-order rate coefficient of the self reaction of CH₃O₂, and $[\text{RO}_2]$ = sum of the concentrations of all organic peroxy radicals.

Specific notes

G2110: The rate coefficient is: `k_HO2_HO2 = (3.0E-13*EXP(460./temp)+2.1E-33*EXP(920./temp)*cair)*(1.+1.4E-21*EXP(2200./temp)*C(ind_H2O))`.
G2117: Converted to Kc [molec-1 cm3] = Kp*R*T/NA, where R is 82.05736 [cm3atmK1mol1].
G2118: Assuming fast equilibrium.

G3109: The rate coefficient is: `k_NO3_NO2 = k_3rd(temp,cair,2.4E-30,3.0,1.6E-12,-0.1,0.6)`.

G3110: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G3203: The rate coefficient is: `k_NO2_HO2 = k_3rd(temp,cair,1.9E-31,3.4,4.0E-12,0.3,0.6)`.

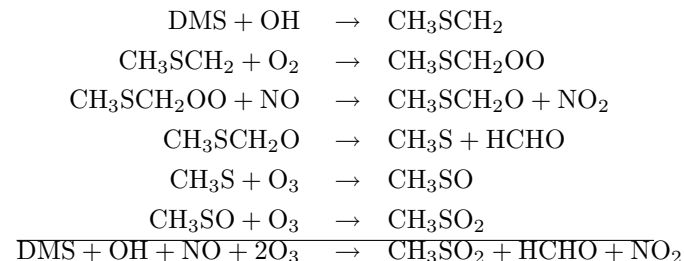
G3206: The rate coefficient is: `k_HNO3_OH = 1.32E-14 * EXP(527./temp) + 1./ (1./ (7.39E-32 * EXP(453./temp)*cair) + 1./ (9.73E-17 * EXP(1910./temp)))`

G3207: The rate coefficient is defined as backward reaction divided by equilibrium constant.

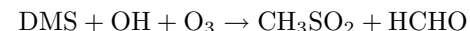
G4103: Sander et al. (2006) recommend a zero product yield for HCHO.

G4109: The same temperature dependence assumed as for CH₃CHO+NO₃. At 298 K, $k = 5.8 \times 10^{-16}$.

G9400a: For the abstraction path, the assumed reaction sequence (omitting H₂O and O₂ as products) according to Yin et al. (1990) is:



Neglecting the effect on O₃ and NO_x, the remaining reaction is:



G9400b: For the addition path, the rate coefficient is: `k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(ind_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind_O2))`.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1001a	UpStTrGJ	$\text{O}_3 + h\nu \rightarrow \text{O}(^1\text{D}) + \text{O}_2$	jx(ip_01D)	Sander et al. (2014)
J1001b	UpStTrGJ	$\text{O}_3 + h\nu \rightarrow \text{O}(^3\text{P}) + \text{O}_2$	jx(ip_03P)	Sander et al. (2014)
J2101	UpStTrGJ	$\text{H}_2\text{O}_2 + h\nu \rightarrow 2 \text{OH}$	jx(ip_H2O2)	Sander et al. (2014)
J3101	UpStTrGJN	$\text{NO}_2 + h\nu \rightarrow \text{NO} + \text{O}(^3\text{P})$	jx(ip_N02)	Sander et al. (2014)
J3103a	UpStTrGJN	$\text{NO}_3 + h\nu \rightarrow \text{NO}_2 + \text{O}(^3\text{P})$	jx(ip_N020)	Sander et al. (2014)
J3103b	UpStTrGJN	$\text{NO}_3 + h\nu \rightarrow \text{NO} + \text{O}_2$	jx(ip_N002)	Sander et al. (2014)
J3104	StTrGJN	$\text{N}_2\text{O}_5 + h\nu \rightarrow \text{NO}_2 + \text{NO}_3$	jx(ip_N205)	Sander et al. (2014)
J3200	TrGJN	$\text{HONO} + h\nu \rightarrow \text{NO} + \text{OH}$	jx(ip_H0N0)	Sander et al. (2014)
J3201	StTrGJN	$\text{HNO}_3 + h\nu \rightarrow \text{NO}_2 + \text{OH}$	jx(ip_HN03)	Sander et al. (2014)
J3202	StTrGJN	$\text{HNO}_4 + h\nu \rightarrow .667 \text{NO}_2 + .667 \text{HO}_2 + .333 \text{NO}_3 + .333 \text{OH}$	jx(ip_HN04)	Sander et al. (2014)
J4100	StTrGJ	$\text{CH}_3\text{OOH} + h\nu \rightarrow \text{HCHO} + \text{OH} + \text{HO}_2$	jx(ip_CH300H)	Sander et al. (2014)
J4101a	StTrGJ	$\text{HCHO} + h\nu \rightarrow \text{H}_2 + \text{CO}$	jx(ip_COH2)	Sander et al. (2014)
J4101b	StTrGJ	$\text{HCHO} + h\nu \rightarrow \text{H} + \text{CO} + \text{HO}_2$	jx(ip_CH0H)	Sander et al. (2014)

General notes

J-values are calculated with an external module (e.g., JVAL) and then supplied to the MECCA chemistry.

Values that originate from the Master Chemical Mechanism (MCM) by Rickard and Pascoe (2009) are translated according in the following way:

$\text{J}(11) \rightarrow \text{jx(ip_COH2)}$
 $\text{J}(12) \rightarrow \text{jx(ip_CHOH)}$
 $\text{J}(15) \rightarrow \text{jx(ip_HOCH2CHO)}$
 $\text{J}(18) \rightarrow \text{jx(ip_MACR)}$
 $\text{J}(22) \rightarrow \text{jx(ip_ACETOL)}$
 $\text{J}(23)+\text{J}(24) \rightarrow \text{jx(ip_MVK)}$
 $\text{J}(31)+\text{J}(32)+\text{J}(33) \rightarrow \text{jx(ip_GLYOX)}$
 $\text{J}(34) \rightarrow \text{jx(ip_MGLYOX)}$

$\text{J}(41) \rightarrow \text{jx(ip_CH300H)}$
 $\text{J}(53) \rightarrow \text{J(isopropyl nitrate)}$
 $\text{J}(54) \rightarrow \text{J(isopropyl nitrate)}$
 $\text{J}(55) \rightarrow \text{J(isopropyl nitrate)}$
 $\text{J}(56)+\text{J}(57) \rightarrow \text{jx(ip_NOA)}$

Specific notes

Table 3: Reversible (Henry’s law) equilibria and irreversible (“heterogenous”) uptake

#	labels	reaction	rate coefficient	reference
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General notes

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in subroutine `mecca_aero_calc_k_ex` in the file `messy_mecca_aero.f90` using accommodation coefficients and Henry’s law constants from chemprop (see `chemprop.pdf`).

For uptake of X ($X = \text{N}_2\text{O}_5$, ClNO_3 , or BrNO_3) and

subsequent reaction with H_2O , Cl^- , and Br^- in H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, and H7602, we define:

$$k_{\text{exf}}(\text{X}) = \frac{k_{\text{mt}}(\text{X}) \times \text{LWC}}{[\text{H}_2\text{O}] + 5 \times 10^2 [\text{Cl}^-] + 3 \times 10^5 [\text{Br}^-]}$$

Here, k_{mt} = mass transfer coefficient, and LWC = liquid water content of the aerosol. The total uptake rate of X is only determined by k_{mt} . The factors only affect

the branching between hydrolysis and the halide reactions. The factor 5×10^2 was chosen such that the chloride reaction dominates over hydrolysis at about $[\text{Cl}^-] > 0.1 \text{ M}$ (see Fig. 3 in Behnke et al. (1997)), i.e. when the ratio $[\text{H}_2\text{O}]/[\text{Cl}^-]$ is less than 5×10^2 . The ratio $5 \times 10^2 / 3 \times 10^5$ was chosen such that the reactions with chloride and bromide are roughly equal for sea water composition (Behnke et al., 1994). These ratios were measured for uptake of N_2O_5 . Here, they are also used for ClNO_3 and BrNO_3 .

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
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General notes

Heterogeneous reaction rates are calculated with an external module (e.g., MECCA_KHET) and then supplied to the MECCA chemistry (see www.messy-interface.org for details)

Table 5: Acid-base and other equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$	reference
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Specific notes

Table 6: Aqueous phase reactions

#	labels	reaction	k_0 [$M^{1-n}s^{-1}$]	$-E_a/R[K]$	reference
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Specific notes

References

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