

IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation – Data Sheet V.A2.12 MD12

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CH₃C(O)CH₃ + mineral oxide (dust) surfaces

Experimental data

Parameter	Temp./K	Reference	Technique/ Comments
<i>Uptake coefficients: γ, γ_0</i>			
$\gamma = 3.7 \times 10^{-4}$ (Adobe clay soil, RH \approx 0)	298	Judeikis, 1982	CRFT (a)
$\gamma > 5.4 \times 10^{-7}$ (Adobe clay soil, RH > 12 %)			
$\gamma_0 = 6.2 \times 10^{-6}$ (SiO ₂)	298	Li et al. 2001	Knudsen-MS (b)
$\gamma_0 = 2.0 \times 10^{-5}$ (α -Al ₂ O ₃)	298		
$\gamma_0 = 1.6 \times 10^{-4}$ (α -Fe ₂ O ₃)	298		
$\gamma_0 = 3.6 \times 10^{-4}$ (TiO ₂)	298		
$\gamma_0 = 1.2 \times 10^{-4}$ (CaO)	298		
<i>Surface partition coefficients: K_{inc}</i>			
$5.3 \times 10^{-11} \exp(6109/T)$ (Quartz, RH = 30 %)	323-373	Goss, 1992	PC-GC (c)
$4.8 \times 10^{-11} \exp(5736/T)$ (Quartz, RH = 50 %)			
$9.1 \times 10^{-12} \exp(5984/T)$ (Quartz, RH = 70 %)			
$\exp(-0.0523 * RH - 4.37)$ (Quartz)			
$1.67 \times 10^{-4} \exp(100-RH * 0.0106)$ (α -Al ₂ O ₃)	333.5	Goss and Eisenreich, 1996	PC-GC (c)
$1.93 \times 10^{-4} \exp(100-RH * 0.0187)$ (α -Fe ₂ O ₃)			
$1.44 \times 10^{-4} \exp(100-RH * 0.0484)$ (Quartz)			
2.36×10^{-2} (Quartz, RH = 40%)	288	Goss and Schwarzenbach, 2002	PC-GC (c)
6.45×10^{-2} (Quartz, RH = 70%)			
2.23×10^{-2} (Quartz, RH = 90%)			
5.29×10^{-3} (α -Al ₂ O ₃ , RH = 40%)			
2.74×10^{-3} (α -Al ₂ O ₃ , RH = 70%)			
2.09×10^{-3} (α -Al ₂ O ₃ , RH = 70%)			
3.76×10^{-3} (CaCO ₃ , RH = 40%)			
2.51×10^{-3} (CaCO ₃ , RH = 70%)			
2.27×10^{-3} (CaCO ₃ , RH = 70%)			

Comments

- (a) Soil sample deposited onto outside of cylindrical flow tube insert from an aqueous slurry and dried under vacuum. Observation of acetone displacement by adding water vapour to previously exposed dry sample and lack of uptake at RH = 12 – 90 % suggest competitive adsorption between acetone and H₂O. Photosensitised desorption of acetone also observed.
- (b) Uptake to bulk samples (1-30 mg) investigated using a Knudsen reactor with pulsed gas inlet and MS analysis of acetone at an initial concentration of 6×10^{10} molecule cm⁻³. The initial uptake coefficients (γ_0) given in the table were calculated using the BET surface area of the sample. Uptake was seen to saturate with exposure time, and time dependent values of γ were

obtained. FTIR and UV/Vis diffuse reflectance analysis of the sample exposed to higher acetone concentrations revealed the presence of reaction products resulting from dehydration reactions (e.g. mesityl oxide).

- (c) Packed column with mineral particles BET-N₂ surface areas used to calculate available surface). K_{linC} in units of cm⁻² / cm⁻³. K_{linC} found to be decrease as temperature and RH increase. The parameterisation in the table is valid for RH > 30 % .

Preferred Values

no recommendation

Comments on Preferred Values

Goss and co-workers have shown that, at equilibrium, the amount of acetone associated with a mineral oxide surface depends on the availability of surface adsorbed water for relative humidity between 30 and 90 % (Goss, 1992, 1994; Goss and Eisenreich, 1994, Goss and Schwarzenbach, 2002), and displays only weak dependence on the nature of the mineral. At RH close to 100 % the partitioning is controlled by dissolution in an aqueous surface film. Goss (1994) presented an algorithm for calculating the equilibrium partitioning, K_{linC} for mineral surfaces such as quartz and kaolinite from given values of temperature and relative humidity: $\ln K = A - \Delta H/R (1/T - 1/323.15) - C(100-RH)$, where $A = -8.18$, $\Delta H = -48.7$ kJmol⁻¹, and $C = -0.0523$ with R in kJmol⁻¹. Most data were obtained at non-ambient temperatures and no information is available for authentic dust samples. For these reasons, no recommendation for K_{linC} is given for the purpose of atmospheric modelling.

References

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Judeikis, H. S., Laboratory measurement of dry deposition of acetone over adobe clay soil, in "Heterogeneous Atmospheric Chemistry", edited by D. R. Schryer, Geophysical Monograph 26, American Geophysical Union, Washington D.C., 1982.
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