Equilibria

Species		K_a or K_h	-ΔH/R (K)	References	Notes
C4 compounds					
Succinic acid					
$CO(OH)CH_2CH_2CO(OH) \leftrightarrow CO(OH)CH_2CH_2CO(O^-) + H^+$	T(1)	$6.2\ 10^{-5}$		Hayne, 2015	
$CO(OH)CH_2CH_2CO(O^-) \leftrightarrow CO(O^-)CH_2CH_2CO(O^-) + H^+$	T(2)	$2.3\ 10^{-6}$		Hayne, 2015	
$CO(OH)CH_2CH(OO^\bullet)CO(OH) \leftrightarrow CO(OH)CH_2CH(OO^\bullet)CO(O^-) + H^+$	T(3)	$6.2\ 10^{-5}$			1 = $K_a(CO(OH)CH_2CH_2CO(OH)/\ CO(OH)CH_2CH_2CO(O^-))$
$CO(OH)CH_2CH(OO^\bullet)CO(OH) \leftrightarrow CO(O^-)CH_2CH(OO^\bullet)CO(OH) + H^+$	T(4)	$6.2\ 10^{-5}$			1 = $K_a(CO(OH)CH_2CH_2CO(OH)/\ CO(OH)CH_2CH_2CO(O^-))$
$CO(OH)CH_2CH(OO^\bullet)CO(O^-) \leftrightarrow CO(O^-)CH_2CH(OO^\bullet)CO(O^-) + H^+$	T(5)	$2.3\ 10^{-6}$			1 = $K_a(CO(OH)CH_2CH_2CO(O^-)/\ CO(O^-)CH_2CH_2CO(O^-))$
Oxaloacetic acid					
$CO(OH)CH_2COCO(OH) \leftrightarrow CO(OH)CH_2COCO(O^-) + H^+$	T(6)	$2.8\ 10^{-3}$		Hayne, 2015	2
$CO(OH)CH_2COCO(OH) \leftrightarrow CO(O^-)CH_2COCO(OH) + H^+$	T(7)	$2.8\ 10^{-3}$		Hayne, 2015	2
$CO(OH)CH_2COCO(O^-) \leftrightarrow CO(O^-)CH_2COCO(O^-) + H^+$	T(8)	$4.3\ 10^{-5}$		Hayne, 2015	
$CO(OH)CH_2COCO(OH) + H_2O \leftrightarrow CO(OH)CH_2C(OH)(OH)CO(OH)$	T(9)	$1.8\ 10^{1}$		Estimated with GROMHE	
$CO(OH)CH_2COCO(O^-) + H_2O \leftrightarrow CO(OH)CH_2C(OH)(OH)CO(O^-)$	T(10)	$1.2\ 10^{-1}$		Estimated with GROMHE	
$CO(O^-)CH_2COCO(OH) + H_2O \leftrightarrow CO(O^-)CH_2C(OH)(OH)CO(OH)$	T(11)	$2.4\ 10^{0}$		Estimated with GROMHE	
$CO(O^-)CH_2COCO(O^-) + H_2O \leftrightarrow CO(O^-)CH_2C(OH)(OH)CO(O^-)$	T(12)	$2.0\ 10^{-2}$		Estimated with GROMHE	
$CO(OH)CH(OO^\bullet)COCO(OH) \leftrightarrow CO(OH)CH(OO^\bullet)COCO(O^-) + H^+$	T(13)	$2.8\ 10^{-3}$			1 = $K_a(CO(OH)CH_2COCO(OH)/\ CO(OH)CH_2COCO(O^-))$
$CO(OH)CH(OO^\bullet)COCO(OH) \leftrightarrow CO(O^-)CH(OO^\bullet)COCO(OH) + H^+$	T(14)	$2.8\ 10^{-3}$			1 = $K_a(CO(OH)CH_2COCO(OH)/\ CO(O^-)CH_2COCO(OH))$
$CO(OH)CH(OO^\bullet)COCO(O^-) \leftrightarrow CO(O^-)CH(OO^\bullet)COCO(O^-) + H^+$	T(15)	$4.3\ 10^{-5}$			1 = $K_a(CO(OH)CH_2COCO(O^-)/\ CO(O^-)CH_2COCO(O^-))$
$CO(OH)CH(OO^\bullet)COCO(OH) + H_2O \leftrightarrow CO(OH)CH(OO^\bullet)C(OH)(OH)CO(OH)$	T(16)	$1.8\ 10^{1}$			3 = $K_h(CO(OH)CH_2COCO(OH)/\ CO(OH)CH_2C(OH)(OH)CO(OH))$
$CO(OH)CH(OO^\bullet)COCO(O^-) + H_2O \leftrightarrow CO(OH)CH(OO^\bullet)C(OH)(OH)CO(O^-)$	T(17)	$1.2\ 10^{-1}$			3 = $K_h(CO(OH)CH_2COCO(O^-)/\ CO(OH)CH_2C(OH)(OH)CO(O^-))$
$CO(O^-)CH(OO^\bullet)COCO(OH) + H_2O \leftrightarrow CO(O^-)CH(OO^\bullet)C(OH)(OH)CO(OH)$	T(18)	$2.4\ 10^{0}$			3 = $K_h(CO(O^-)CH_2COCO(OH)/\ CO(O^-)CH_2C(OH)(OH)CO(OH))$
$CO(O^-)CH(OO^\bullet)COCO(O^-) + H_2O \leftrightarrow CO(O^-)CH(OO^\bullet)C(OH)(OH)CO(O^-)$	T(19)	$2.0\ 10^{-2}$			3 = $K_h(CO(O^-)CH_2COCO(O^-)/\ CO(O^-)CH_2C(OH)(OH)CO(O^-))$
Malic acid					
$CO(OH)CH_2CH(OH)CO(OH) \leftrightarrow CO(OH)CH_2CH(OH)CO(O^-) + H^+$	T(20)	$4.0\ 10^{-4}$		Hayne, 2015	2

Species		K_a or K_h	-ΔH/R (K)	References	Notes
$CO(OH)CH_2CH(OH)CO(OH) \leftrightarrow CO(O^-)CH_2CH(OH)CO(OH) + H^+$	T(21)	$4.0\ 10^{-4}$		Hayne, 2015	2
$CO(OH)CH_2CH(OH)CO(O^-) \leftrightarrow CO(O^-)CH_2CH(OH)CO(O^-) + H^+$	T(22)	$7.8\ 10^{-6}$		Hayne, 2015	
$CO(OH)CH_2C(OH)(OO^\bullet)CO(OH) \leftrightarrow CO(OH)CH_2C(OH)(OO^\bullet)CO(O^-) + H^+$	T(23)	$4.0\ 10^{-4}$			1 = $K_a(CO(OH)CH_2CH(OH)CO(OH)/ CO(OH)CH_2CH(OH)CO(O^-))$
$CO(OH)CH_2C(OH)(OO^\bullet)CO(OH) \leftrightarrow CO(O^-)CH_2C(OH)(OO^\bullet)CO(OH) + H^+$	T(24)	$4.0\ 10^{-4}$			1 = $K_a(CO(OH)CH_2CH(OH)CO(OH)/ CO(O^-)CH_2CH(OH)CO(OH))$
$CO(OH)CH_2C(OH)(OO^\bullet)CO(O^-) \leftrightarrow CO(O^-)CH_2C(OH)(OO^\bullet)CO(O^-) + H^+$	T(25)	$7.8\ 10^{-6}$			1 = $K_a(CO(OH)CH_2CH(OH)CO(O^-)/ CO(O^-)CH_2CH(OH)CO(O^-))$
Tartric acid					
$CO(OH)CH(OH)CH(OH)CO(OH) \leftrightarrow CO(OH)CH(OH)CH(OH)CO(O^-) + H^+$	T(26)	$9.3\ 10^{-4}$		Hayne, 2015	
$CO(OH)CH(OH)CH(OH)CO(O^-) \leftrightarrow CO(O^-)CH(OH)CH(OH)CO(O^-) + H^+$	T(27)	$4.3\ 10^{-5}$		Hayne, 2015	
$CO(OH)C(OH)(OO^\bullet)CH(OH)CO(OH) \leftrightarrow CO(OH)CH(OH)C(OH)(OO^\bullet)CO(O^-) + H^+$	T(28)	$9.3\ 10^{-4}$			1 = $K_a(CO(OH)CH(OH)CH(OH)CO(OH)/ CO(OH)CH(OH)CH(OH)CO(O^-))$
$CO(OH)C(OH)(OO^\bullet)CH(OH)CO(OH) \leftrightarrow CO(O^-)CH(OH)C(OH)(OO^\bullet)CO(OH) + H^+$	T(29)	$9.3\ 10^{-4}$			1 = $K_a(CO(OH)CH(OH)CH(OH)CO(OH)/ CO(OH)CH(OH)CH(OH)CO(O^-))$
$CO(OH)CH(OH)C(OH)(OO^\bullet)CO(O^-) \leftrightarrow CO(O^-)CH(OH)C(OH)(OO^\bullet)CO(O^-) + H^+$	T(30)	$4.3\ 10^{-5}$			1 = $K_a(CO(OH)CH(OH)CH(OH)CO(O^-)/ CO(O^-)CH(OH)CH(OH)CO(O^-))$
Fumaric acid					
$CO(OH)CH=CHCO(OH) \leftrightarrow CO(OH)CH=CHCO(O^-) + H^+$	T(31)	$9.5\ 10^{-4}$		Hayne, 2015	
$CO(OH)CH=CHCO(O^-) \leftrightarrow CO(O^-)CH=CHCO(O^-) + H^+$	T(32)	$4.2\ 10^{-5}$		Hayne, 2015	
$CO(OH)CH(OH)CH(OO^\bullet)CO(OH) \leftrightarrow CO(O^-)CH(OH)CH(OO^\bullet)CO(OH)$	T(33)	$9.5\ 10^{-4}$			1 = $K_a(CO(OH)CH=CHCO(OH)/ CO(OH)CH=CHCO(O^-))$
$CO(OH)CH(OH)CH(OO^\bullet)CO(OH) \leftrightarrow CO(O^-)CH(OO^\bullet)CH(OH)CO(OH)$	T(34)	$9.5\ 10^{-4}$			1 = $K_a(CO(OH)CH=CHCO(OH)/ CO(OH)CH=CHCO(O^-))$
$CO(O^-)CH(OH)CH(OO^\bullet)CO(OH) \leftrightarrow CO(O^-)CH(OH)CH(OO^\bullet)CO(O^-)$	T(35)	$4.2\ 10^{-5}$			1 = $K_a(CO(O^-)CH=CHCO(O^-)/ CO(O^-)CH=CHCO(O^-))$
Maleic acid					
$CO(OH)CH=CHCO(OH) \leftrightarrow CO(OH)CH=CHCO(O^-) + H^+$	T(36)	$1.2\ 10^{-2}$		Hayne, 2015	
$CO(OH)CH=CHCO(O^-) \leftrightarrow CO(O^-)CH=CHCO(O^-) + H^+$	T(37)	$5.9\ 10^{-7}$		Hayne, 2015	

1 - For peroxy radicals, we assumed that the acidity constant is similar to the parent species.
2 - We suppose that the two monoanions present similar K_a.
3 - For peroxy radicals, we assumed that the hydration constant is similar to the parent species.

References:

Hayne, W. M.: CRC Handbook of Chemistry and Physics, Boca Raton, FL, CRC Press, 96e ed., 2677 p., 2015.

Henry's law constants

Species		H (298K) ($M\ atm^{-1}$)	-ΔH/R (K)	References	Notes
C4 compounds					
Succinic acid					
$CO(OH)CH_2CH_2CO(OH)$	T(1)	$5.2\ 10^8$	6014	Estimated	1 - 2
Oxaloacetic acid					
$CO(OH)CH_2COCO(OH)$	T(2)	$5.8\ 10^8$	6014	Estimated	1 - 2 - 3
Malic acid					
$CO(OH)CH_2CH(OH)CO(OH)$	T(3)	$4.5\ 10^8$	6014	Estimated	1 - 2
Tartric acid					
$CO(OH)CH(OH)CH(OH)CO(OH)$	T(4)	$2.7\ 10^9$	6014	Estimated	1 - 2
Fumaric/maleic acid					
$CO(OH)CH(OH)CH(OH)CO(OH)$	T(5)	$4.7\ 10^7$	6014	Estimated	1 - 2

1 - Estimated by the SAR GROMHE (Raventos-Duran et al., 2010).
2 - When unavailable, the temperature dependence (enthalpy of dissolution) is set at 50 $kJ\ mol^{-1}$; -ΔH/R = 6014 K.
3 - Effective Henry's law constant.

References:

Raventos-Duran, T., Camredon, M., Valorso, R., Mouchel-Vallon, C., and Aumont, B.: Structure-activity relationships to estimate the effective Henry's law constants of organics of atmospheric interest, Atmos. Chem. Phys., 10, 7643-7654, 2010.

Accommodation coefficients

Species	α (298K)	-ΔH (J/mol)	-ΔS (J/mol/K)	References	Notes
C4 compounds	1				
Succinic acid					
$CO(OH)CH_2CH_2CO(OH)$	$5.0\ 10^{-2}$			Estimated	2
Oxaloacetic acid					
$CO(OH)CH_2COCO(OH)$	$5.0\ 10^{-2}$			Estimated	2
Malic acid					
$CO(OH)CH_2CH(OH)CO(OH)$	$5.0\ 10^{-2}$			Estimated	2
Tartric acid					
$CO(OH)CH(OH)CH(OH)CO(OH)$	$5.0\ 10^{-2}$			Estimated	2
Fumaric/maleic acid					
$CO(OH)CH(OH)CH(OH)CO(OH)$	$5.0\ 10^{-2}$			Estimated	2

1 - α can be calculated with ΔH and ΔS; this allows considering the temperature dependency of α following Jayne et al. (1991): $\frac{\alpha}{1-\alpha} = \exp\left(\frac{-\Delta G}{RT}\right)$; $\Delta G = \Delta H - T\Delta S$

2 - Estimated equal $5.0\ 10^{-2}$ following Lelieveld and Crutzen (1991) and Davidovits et al. (2011).

References:

Davidovits, P., Kolb, C. E., Williams, L. R., Jayne, J. T., and Worsnop, D. R.: Update 1 of: Mass accommodation and chemical reactions at gas–liquid interfaces, Chem. Rev., 111, 2011.

Jayne, J. T., Duan, S. X., Davidovits, P., Worsnop, D. R., Zahniser, M. S., and Kolb, C. E. Uptake of gas-phase alcohol and organic acid molecules by water surfaces, J. Phys. Chem., 95, 6329, 1991.

Lelieveld, J., and Crutzen, P. J.: The role of clouds in tropospheric photochemistry, J. Atmos. Chem., 12, 229-267, 1991.