



#### Equilibrium constants for hydrolysis and associated equilibria in critical compilations

## Iron(II)

Equilibrium reactions	$\lg K$ at infinite dilution and $T = 298 \text{ K}$		
	Baes and Mesmer, 1976	Lemire et al., 2013	Brown and Ekberg, 2016
$Fe^{2+} + H_2O \rightleftharpoons FeOH^+ + H^+$	-9.5	-9.1 ± 0.4	-9.43 ± 0.10
$Fe^{2+} + 2 H_2O \rightleftharpoons Fe(OH)_2 + 2 H^+$	-20.6	-21.2±1.1	-20.52 ± 0.08
$Fe^{2+} + 3 H_2O \rightleftharpoons Fe(OH)_3^- + 3 H^+$	-31	-34.3±0.2	-32.68 ± 0.15
$Fe^{2+} + 4 H_2O \rightleftharpoons Fe(OH)_4^2 + 4 H^+$	-46		
$Fe(OH)_2(s) +2 H^+ \rightleftharpoons Fe^{2+} + 2 H_2O$	12.85	12.5 ± 0.02	12.27 ± 0.88

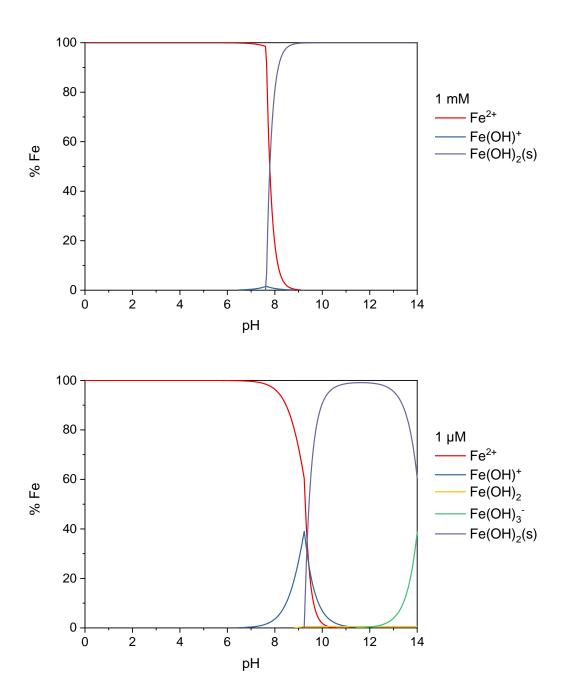
C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, p. 235.

P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 573–585.

R.J. Lemire, U. Berner, C. Musikas, D.A. Palmer, P.Taylor, O. Tochiyama, Chemical Thermodynamics Volume 13a in the OECD Nuclear Energy Agency (NEA) Chemical Thermodynamics series, Chemical Thermodynamics of Iron, Part 1, 2013.

## Distribution diagrams

These diagrams have been computed at two Fe(II) concentrations (1 mM =  $1x10^{-3}$  mol L<sup>-1</sup> and 1  $\mu$ M =  $1x10^{-6}$  mol L<sup>-1</sup>) with the 'best' equilibrium constants above (in green). Calculations assume T = 298 K for the limiting case of zero ionic strength (*i.e.*, even neglecting plotted ions).





#### Equilibrium constants for hydrolysis and associated equilibria in critical compilations

# Iron(III)

Equilibrium reactions	$\lg K$ at infinite dilution and $T = 298 \text{ K}$		
	Baes and Mesmer, 1976	Lemire et al., 2013	Brown and Ekberg, 2016
$Fe^{3+} + H_2O \rightleftharpoons FeOH^{2+} + H+$	-2.19	-2.15 ± 0.07	-2.20 ± 0.02
$Fe^{3+} + 2 H_2O \rightleftharpoons Fe(OH)_2^+ + 2 H^+$	-5.67	-4.8 ± 0.4	-5.71 ± 0.10
$Fe^{3+} + 3 H_2O \rightleftharpoons Fe(OH)_3 + 3 H^+$	<-12	<-14	-12.42 ± 0.20
$Fe^{3+} + 4 H_2O \rightleftharpoons Fe(OH)_4^- + 4 H^+$	-21.6	-21.5 ± 0.5	-21.60 ± 0.23
2 Fe <sup>3+</sup> + 2 H <sub>2</sub> O $\rightleftharpoons$ Fe <sub>2</sub> (OH) <sub>2</sub> <sup>4+</sup> + 2 H <sup>+</sup>	-2.95	-2.91 ± 0.07	-2.91 ± 0.07
$3 \text{ Fe}^{3+} + 4 \text{ H}_2\text{O} \rightleftharpoons \text{Fe}_3(\text{OH})_4^{5+} + 4 \text{ H}^+$	-6.3		-6.3 ± 0.1
Fe(OH) <sub>3</sub> (s) +3 H <sup>+</sup> $\rightleftharpoons$ Fe <sup>3+</sup> + 3 H <sub>2</sub> O 2-line ferrihydrite	2.5	3.5	3.50 ± 0.20
$Fe(OH)_3(s) \rightleftharpoons Fe^{3+} + 3 OH^-$ 6-line ferrihydrite		-38.97 ± 0.64	
$\alpha$ -FeOOH(s)+ 3 H <sup>+</sup> $\rightleftharpoons$ Fe <sup>3+</sup> + 2 H <sub>2</sub> O goethite	0.5		0.33 ± 0.10
$\alpha$ -FeOOH + H <sub>2</sub> O $\rightleftharpoons$ Fe <sup>3+</sup> + 3 OH <sup>-</sup> goethite		-41.83 ± 0.37	
0.5 $\alpha$ -Fe <sub>2</sub> O <sub>3</sub> (s)+ 3 H <sup>+</sup> $\rightleftharpoons$ Fe <sup>3+</sup> + 1.5 H <sub>2</sub> O hematite			0.36 ± 0.40

$0.5 \alpha$ -Fe <sub>2</sub> O <sub>3</sub> + 1.5 H <sub>2</sub> O $\rightleftharpoons$ Fe <sup>3+</sup> + 3 OH <sup>-</sup> hematite	-42.05 ± 0.26	
0.5 γ-Fe <sub>2</sub> O <sub>3</sub> (s) + 3 H <sup>+</sup> $\rightleftharpoons$ Fe <sup>3+</sup> + 1.5 H <sub>2</sub> O maghemite		1.61 ± 0.61
$0.5  \gamma\text{-Fe}_2\text{O}_3 + 1.5  \text{H}_2\text{O} \rightleftharpoons \text{Fe}^{3+} + 3  \text{OH}^-$ maghemite	-40.59 ± 0.29	
$\alpha$ -FeOOH(s)+ 3 H <sup>+</sup> $\rightleftharpoons$ Fe <sup>3+</sup> + 2 H <sub>2</sub> O lepidocrocite		1.85 ± 0.37
$\gamma$ -FeOOH + H <sub>2</sub> O $\rightleftharpoons$ Fe <sup>3+</sup> + 3 OH <sup>-</sup> lepidocrocite	-40.13 ± 0.37	
Fe(OH) <sub>3</sub> (s) + 3 H <sup>+</sup> $\rightleftharpoons$ Fe <sup>3+</sup> + 3 H <sub>2</sub> O magnetite		-12.26 ± 0.26

C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, p. 235.

P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 585–620.

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