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Equilibrium constants for hydrolysis and associated equilibria in critical compilations

Zirconium

Equilibrium reactions	lg*K* at infinite dilution and *T* = 298 K		
	Baes and Mesmer, 1976	Thoenen et al., 2014	Brown and Ekberg, 2016
$Zr^{4+} + H_2O \rightleftharpoons ZrOH^{3+} + H^+$	0.3	0.32 ± 0.22	0.12 ± 0.12
$Zr^{4+} + 2\ H_2O \rightleftharpoons Zr(OH)_2^{2+} + 2\ H^+$	(−1.7)*	0.98 ± 1.06*	−0.18 ± 0.17*
$Zr^{4+} + 3\ H_2O \rightleftharpoons Zr(OH)_3^{+} + 3\ H^+$	(−5.1)		
$Zr^{4+} + 4\ H_2O \rightleftharpoons Zr(OH)_4 + 4\ H^+$	–9.7*	–2.19 ± 0.70*	−4.53 ± 0.37*
$Zr^{4+} + 5\ H_2O \rightleftharpoons Zr(OH)_5^{-} + 5\ H^+$	–16.0		
$Zr^{4+} + 6\ H_2O \rightleftharpoons Zr(OH)_6^{2-} + 6\ H^+$		–29± 0.70	–30.5 ± 0.3
$3\ Zr^{4+} + 4\ H_2O \rightleftharpoons Zr_3(OH)_4^{8+} + 4\ H^+$	–0.6	0.4 ± 0.3	0.90 ± 0.18
$3\ Zr^{4+} + 5\ H_2O \rightleftharpoons Zr_3(OH)_5^{7+} + 5\ H^+$	3.70		
$3\ Zr^{4+} + 9\ H_2O \rightleftharpoons Zr_3(OH)_9^{3+} + 9\ H^+$		12.19 ± 0.20	12.19 ± 0.20
$4\ Zr^{4+} + 8\ H_2O \rightleftharpoons Zr_4(OH)_8^{8+} + 8\ H^+$	6.0	6.52 ± 0.05	6.52 ± 0.05
$4\ Zr^{4+} + 15\ H_2O \rightleftharpoons Zr_4(OH)_{15}^{+} + 15\ H^+$		12.58± 0.24	
$4\ Zr^{4+} + 16\ H_2O \rightleftharpoons Zr_4(OH)_{16} + 16\ H^+$		8.39± 0.80	
$ZrO_2(s) + 4\ H^+ \rightleftharpoons Zr^{4+} + 2\ H_2O$	–1.9*		–5.37 ± 0.42*

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ZrO_2(s, baddeleyite) + 4 H^+ ⇌ Zr^{4+} + 2 H_2O		–7 ± 1.6	
$Zr(OH)_4$(am) + 4 H^+ ⇌ Zr^{4+} + 4 H_2O		–3.24± 0.10	–2.97 ± 0.18

*Errors in compilations concerning equilibrium and/or data elaboration. Data not recommended. It is strongly suggested to refer to the original papers.

C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, pp. 158.

P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 442–460.

T. Thoenen, W. Hummel, U. Berner and E. Curti, The PSI/Nagra Chemical Thermodynamic Database 12/07, 2014.

Distribution diagrams

These diagrams have been computed at two Zr concentrations (1 mM = $1x10^{-3}$ mol L^{-1} and 1 μM = $1x10^{-6}$ mol L^{-1}) 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).