

Equilibrium constants for hydrolysis and associated equilibria in critical compilations

Zirconium

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

$\text{ZrO}_2(\text{s, baddeleyite}) + 4 \text{H}^+ \rightleftharpoons \text{Zr}^{4+} + 2 \text{H}_2\text{O}$		-7 ± 1.6	
$\text{Zr}(\text{OH})_4(\text{am}) + 4 \text{H}^+ \rightleftharpoons \text{Zr}^{4+} + 4 \text{H}_2\text{O}$		-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 = 1×10^{-3} mol L⁻¹ and 1 μ M = 1×10^{-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).

