

Equilibrium constants for hydrolysis and associated equilibria in critical compilations

Uranium(IV)

Equilibrium reactions	lgK at infinite dilution and T = 298 K			
	Baes and Mesmer, 1976	Thoenen et al., 2014	Brown and Ekberg, 2016	Grenthe et al., 2020
$\text{U}^{4+} + \text{H}_2\text{O} \rightleftharpoons \text{UOH}^{3+} + \text{H}^+$	-0.65	-0.54 ± 0.06	-0.58 ± 0.08	-0.54 ± 0.06
$\text{U}^{4+} + 2 \text{H}_2\text{O} \rightleftharpoons \text{U}(\text{OH})_2^{2+} + 2 \text{H}^+$	(-2.6)	-1.1 ± 1.0	-1.4 ± 0.2	-1.9 ± 0.2
$\text{U}^{4+} + 3 \text{H}_2\text{O} \rightleftharpoons \text{U}(\text{OH})_3^+ + 3 \text{H}^+$	(-5.8)	-4.7 ± 1.0	-5.1 ± 0.3	-5.2 ± 0.4
$\text{U}^{4+} + 4 \text{H}_2\text{O} \rightleftharpoons \text{U}(\text{OH})_4 + 4 \text{H}^+$	(-10.3)	-10.0 ± 1.4	-10.4 ± 0.5	-10.0 ± 1.4
$\text{U}^{4+} + 5 \text{H}_2\text{O} \rightleftharpoons \text{U}(\text{OH})_5^- + 5 \text{H}^+$	-16.0			
$\text{UO}_2(\text{am, hyd}) + 4 \text{H}^+ \rightleftharpoons \text{U}^{4+} + 2 \text{H}_2\text{O}$		1.5 ± 1.0		
$\text{UO}_2(\text{am,hyd}) + 2 \text{H}_2\text{O} \rightleftharpoons \text{U}^{4+} + 4 \text{OH}^-$			-54.500 ± 1.000	-54.500 ± 1.000
$\text{UO}_2(\text{c}) + 4 \text{H}^+ \rightleftharpoons \text{U}^{4+} + 2 \text{H}_2\text{O}$	-1.8			
$\text{UO}_2(\text{c}) + 2 \text{H}_2\text{O} \rightleftharpoons \text{U}^{4+} + 4 \text{OH}^-$				-60.860 ± 1.000

C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, p. 181.

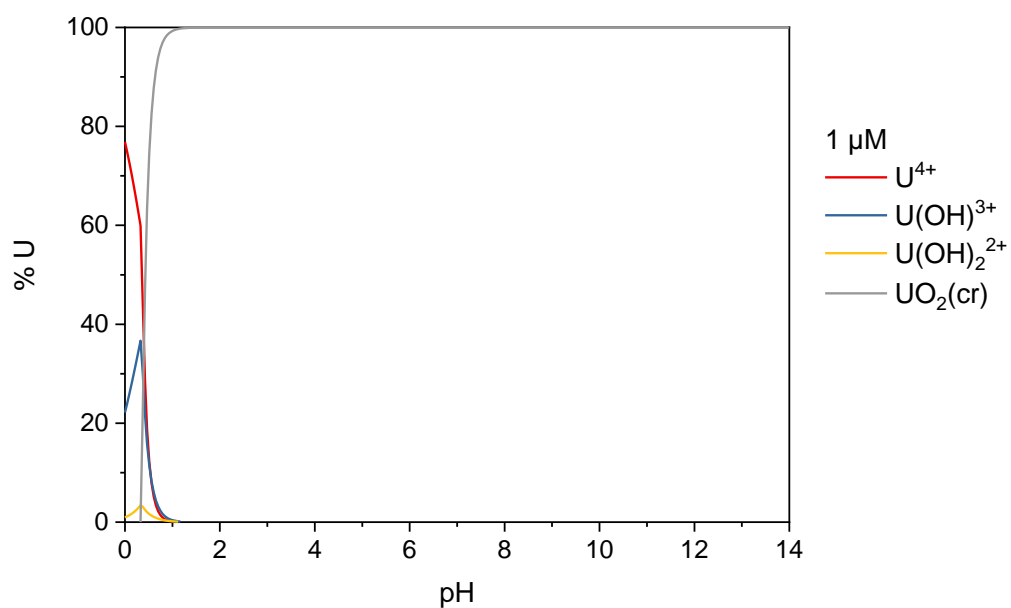
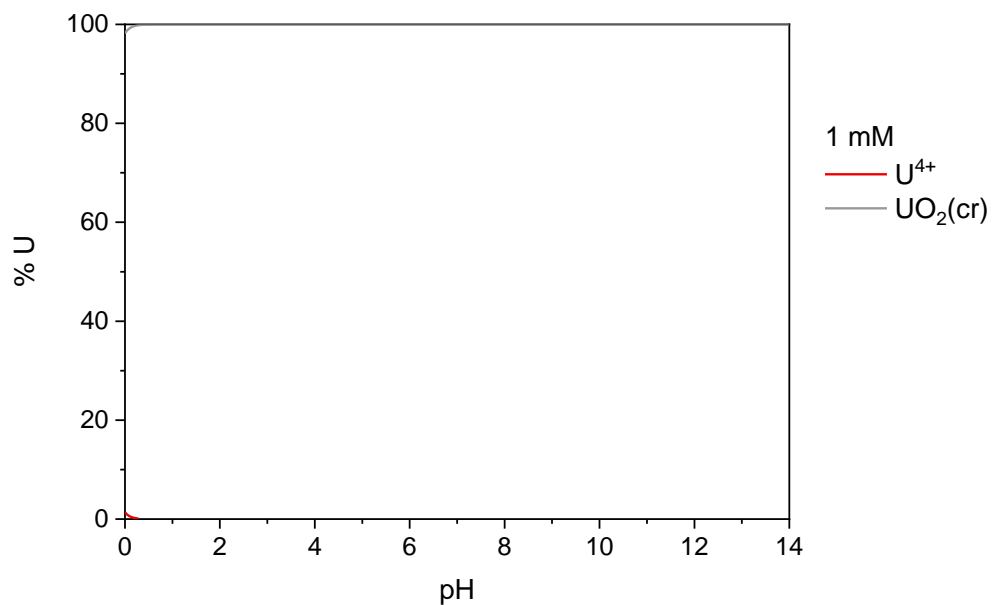
P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 336–349.

I. Grenthe, X. Gaona, A.V. Plyasunov, L. Rao, W.H. Runde, B. Grambow, R.J.M. Konings, A.L. Smith and E.E. Moore, Second Update on the Chemical Thermodynamics of Uranium, Neptunium, Plutonium, Americium and Technetium, OECD Pub., 2020.

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

Distribution diagrams

These diagrams have been computed at two U(IV) concentrations ($1 \text{ mM} = 1 \times 10^{-3} \text{ mol L}^{-1}$ and $1 \text{ }\mu\text{M} = 1 \times 10^{-6} \text{ mol L}^{-1}$) with the 'best' equilibrium constants above (in green). Calculations assume $T = 298 \text{ K}$ for the limiting case of zero ionic strength (*i.e.*, even neglecting plotted ions).



Equilibrium constants for hydrolysis and associated equilibria in critical compilations

Uranium(VI)

Equilibrium reactions	lgK at infinite dilution and $T = 298 \text{ K}$				
	Baes and Mesmer, 1976	Grenthe et al., 1992	NIST46	Brown and Ekberg, 2016	Grenthe et al., 2020
$\text{UO}_2^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{UO}_2(\text{OH})^+ + \text{H}^+$	-5.8	-5.2 ± 0.3	-5.9 ± 0.1	-5.13 ± 0.04	$-5.2_5 \pm 0.2_4$
$\text{UO}_2^{2+} + 2 \text{H}_2\text{O} \rightleftharpoons \text{UO}_2(\text{OH})_2 + 2 \text{H}^+$		≤ -10.3		$-12.1_5 \pm 0.2_0$	-12.15 ± 0.07
$\text{UO}_2^{2+} + 3 \text{H}_2\text{O} \rightleftharpoons \text{UO}_2(\text{OH})_3^- + 3 \text{H}^+$		-19.2 ± 0.4		$-20.2_5 \pm 0.4_2$	$-20.2_5 \pm 0.4_2$
$\text{UO}_2^{2+} + 4 \text{H}_2\text{O} \rightleftharpoons \text{UO}_2(\text{OH})_4^{2-} + 4 \text{H}^+$		-33 ± 2		$-32.4_0 \pm 0.6_8$	$-32.4_0 \pm 0.6_8$
$2 \text{UO}_2^{2+} + 2 \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_2(\text{OH})_2^{2+} + 2 \text{H}^+$	-5.62	-5.62 ± 0.04	-5.58 ± 0.04	-5.68 ± 0.05	-5.62 ± 0.08
$3 \text{UO}_2^{2+} + 5 \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_3(\text{OH})_5^+ + 5 \text{H}^+$	-15.63	$-15.5_5 \pm 0.1_2$	-15.6	$-15.7_5 \pm 0.1_2$	$-15.5_5 \pm 0.1_2$

$3 \text{UO}_2^{2+} + 4 \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_3(\text{OH})_4^{2+} + 4 \text{H}^+$	(-11.75)	-11.9 ± 0.3		-11.78 ± 0.05	-11.9 ± 0.3
$3 \text{UO}_2^{2+} + 7 \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_3(\text{OH})_7^- + 7 \text{H}^+$		-31 ± 2.0		-32.2 ± 0.8	-32.2 ± 0.8
$4 \text{UO}_2^{2+} + 7 \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_4(\text{OH})_7^+ + 7 \text{H}^+$		-21.9 ± 1.0		-22.1 ± 0.2	-21.9 ± 1.0
$2 \text{UO}_2^{2+} + \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_2(\text{OH})_3^{3+} + \text{H}^+$		-2.7 ± 1.0			-2.7 ± 1.0
$\text{UO}_2(\text{OH})_2(\text{s}) + 2\text{H}^+ \rightleftharpoons \text{UO}_2^{2+} + 2 \text{H}_2\text{O}$	5.6		6.0	4.81 ± 0.20	
$\text{UO}_3 \cdot 2\text{H}_2\text{O}(\text{cr}) + 2\text{H}^+ \rightleftharpoons \text{UO}_2^{2+} + 3 \text{H}_2\text{O}$					5.350 ± 0.130

C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, p. 182.

P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 350–379.

I. Grenthe, J. Fuger, R.J.M. Konings, R.J. Lemire, A.B. Muller, C. Nguyen-Trung and H. Wanner, Chemical Thermodynamics of Uranium, Chemical Vol 1, OECD Publishing, Paris, 1992.

I. Grenthe, X. Gaona, A.V. Plyasunov, L. Rao, W.H. Runde, B. Grambow, R.J.M. Konings, A.L. Smith and E.E. Moore, Second Update on the Chemical Thermodynamics of Uranium, Neptunium, Plutonium, Americium and Technetium, OECD Publishing, Paris, 2020.

NIST46, NIST Critically Selected Stability Constants of Metal Complexes: Version 8.0. Available at: www.nist.gov/srd/nist46

Distribution diagrams

These diagrams have been computed at two U(VI) 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).

