

## 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
$U^{4+} + H_2O \rightleftharpoons UOH^{3+} + H^+$	-0.65	$-0.54 \pm 0.06$	$-0.58 \pm 0.08$	$-0.54 \pm 0.06$
$U^{4+} + 2 H_2O \rightleftharpoons U(OH)_2^{2+} + 2 H^+$	(-2.6)	$-1.1 \pm 1.0$	$-1.4 \pm 0.2$	$-1.9 \pm 0.2$
$U^{4+} + 3 H_2O \rightleftharpoons U(OH)_3^+ + 3 H^+$	(-5.8)	$-4.7 \pm 1.0$	$-5.1 \pm 0.3$	$-5.2 \pm 0.4$
$U^{4+} + 4 H_2O \rightleftharpoons U(OH)_4 + 4 H^+$	(-10.3)	$-10.0 \pm 1.4$	$-10.4 \pm 0.5$	$-10.0 \pm 1.4$
$U^{4+} + 5 H_2O \rightleftharpoons U(OH)_5^- + 5 H^+$	-16.0			
$UO_2(\text{am, hyd}) + 4 H^+ \rightleftharpoons U^{4+} + 2 H_2O$		$1.5 \pm 1.0$		
$UO_2(\text{am,hyd}) + 2 H_2O \rightleftharpoons U^{4+} + 4 OH^-$			$-54.500 \pm 1.000$	$-54.500 \pm 1.000$
$UO_2(\text{c}) + 4 H^+ \rightleftharpoons U^{4+} + 2 H_2O$	-1.8			
$UO_2(\text{c}) + 2 H_2O \rightleftharpoons U^{4+} + 4 OH^-$				$-60.860 \pm 1.000$

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

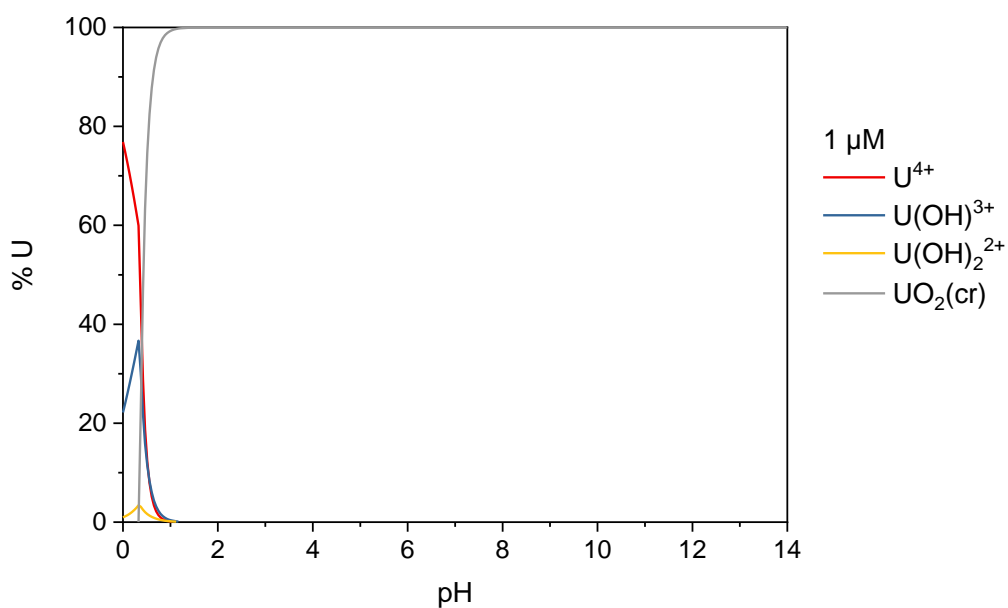
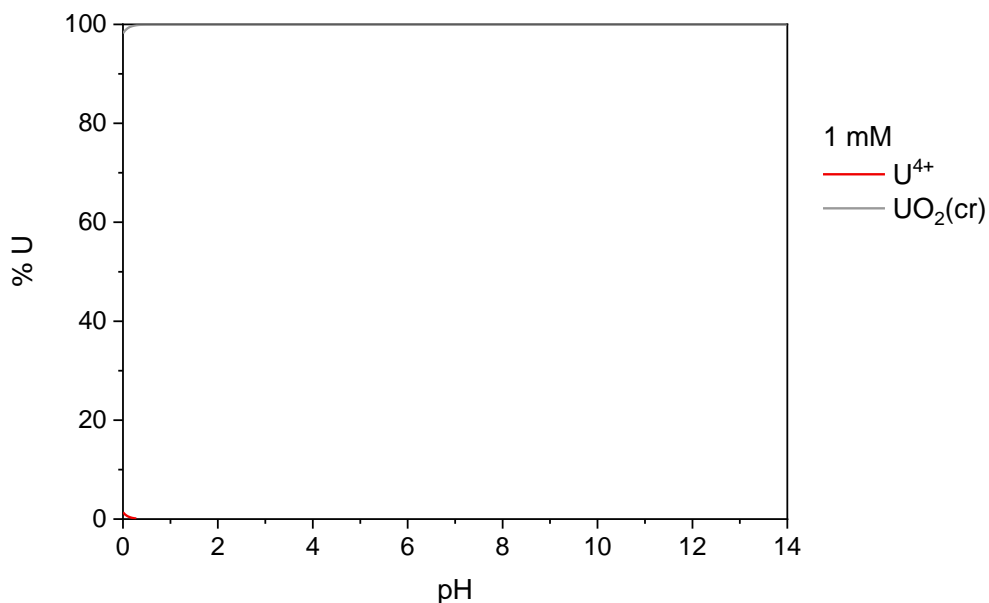
P.L. Brown and C. Ekberg, *Hydrolysis of Metal Ions*. Wiley, 2016, pp. 336–349.

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 mM =  $1 \times 10^{-3}$  mol L<sup>-1</sup> and 1  $\mu$ M =  $1 \times 10^{-6}$  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

# 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	$-5.2 \pm 0.3$	$-5.9 \pm 0.1$	$-5.13 \pm 0.04$	$-5.2_5 \pm 0.2_4$
$\text{UO}_2^{2+} + 2 \text{H}_2\text{O} \rightleftharpoons \text{UO}_2(\text{OH})_2 + 2 \text{H}^+$		$\leq -10.3$		$-12.1_5 \pm 0.2_0$	$-12.15 \pm 0.07$
$\text{UO}_2^{2+} + 3 \text{H}_2\text{O} \rightleftharpoons \text{UO}_2(\text{OH})_3^- + 3 \text{H}^+$		$-19.2 \pm 0.4$		$-20.2_5 \pm 0.4_2$	$-20.2_5 \pm 0.4_2$
$\text{UO}_2^{2+} + 4 \text{H}_2\text{O} \rightleftharpoons \text{UO}_2(\text{OH})_4^{2-} + 4 \text{H}^+$		$-33 \pm 2$		$-32.4_0 \pm 0.6_8$	$-32.4_0 \pm 0.6_8$
$2 \text{UO}_2^{2+} + 2 \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_2(\text{OH})_2^{2+} + 2 \text{H}^+$	-5.62	$-5.62 \pm 0.04$	$-5.58 \pm 0.04$	$-5.68 \pm 0.05$	$-5.62 \pm 0.08$
$3 \text{UO}_2^{2+} + 5 \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_3(\text{OH})_5^+ + 5 \text{H}^+$	-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)	$-11.9 \pm 0.3$		$-11.78 \pm 0.05$	$-11.9 \pm 0.3$
$3 \text{UO}_2^{2+} + 7 \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_3(\text{OH})_7^- + 7 \text{H}^+$		$-31 \pm 2.0$		$-32.2 \pm 0.8$	$-32.2 \pm 0.8$
$4 \text{UO}_2^{2+} + 7 \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_4(\text{OH})_7^+ + 7 \text{H}^+$		$-21.9 \pm 1.0$		$-22.1 \pm 0.2$	$-21.9 \pm 1.0$
$2 \text{UO}_2^{2+} + \text{H}_2\text{O} \rightleftharpoons (\text{UO}_2)_2(\text{OH})_3^+ + \text{H}^+$		$-2.7 \pm 1.0$			$-2.7 \pm 1.0$
$\text{UO}_2(\text{OH})_2(\text{s}) + 2\text{H}^+ \rightleftharpoons \text{UO}_2^{2+} + 2 \text{H}_2\text{O}$	5.6		6.0	$4.81 \pm 0.20$	
$\text{UO}_3 \cdot 2\text{H}_2\text{O}(\text{cr}) + 2\text{H}^+ \rightleftharpoons \text{UO}_2^{2+} + 3 \text{H}_2\text{O}$					$5.350 \pm 0.130$

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](http://www.nist.gov/srd/nist46)

# Distribution diagrams

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