

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

# Plutonium(III)

Equilibrium reactions	lgK at infinite dilution and $T = 298\text{ K}$			
	Baes and Mesmer, 1976	NIST46	Brown and Ekberg, 2016	Grenthe et al., 2020
$\text{Pu}^{3+} + \text{H}_2\text{O} \rightleftharpoons \text{Pu}(\text{OH})^{2+} + \text{H}^+$		-7.0	$-6.9 \pm 0.2$	$-6.9 \pm 0.3$
$\text{Pu}^{3+} + 3 \text{H}_2\text{O} \rightleftharpoons \text{Pu}(\text{OH})_3(\text{cr}) + 3 \text{H}^+$	-19.65		$-15.8 \pm 0.8$	$-15 \pm 1$

C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, pp. 186–187.

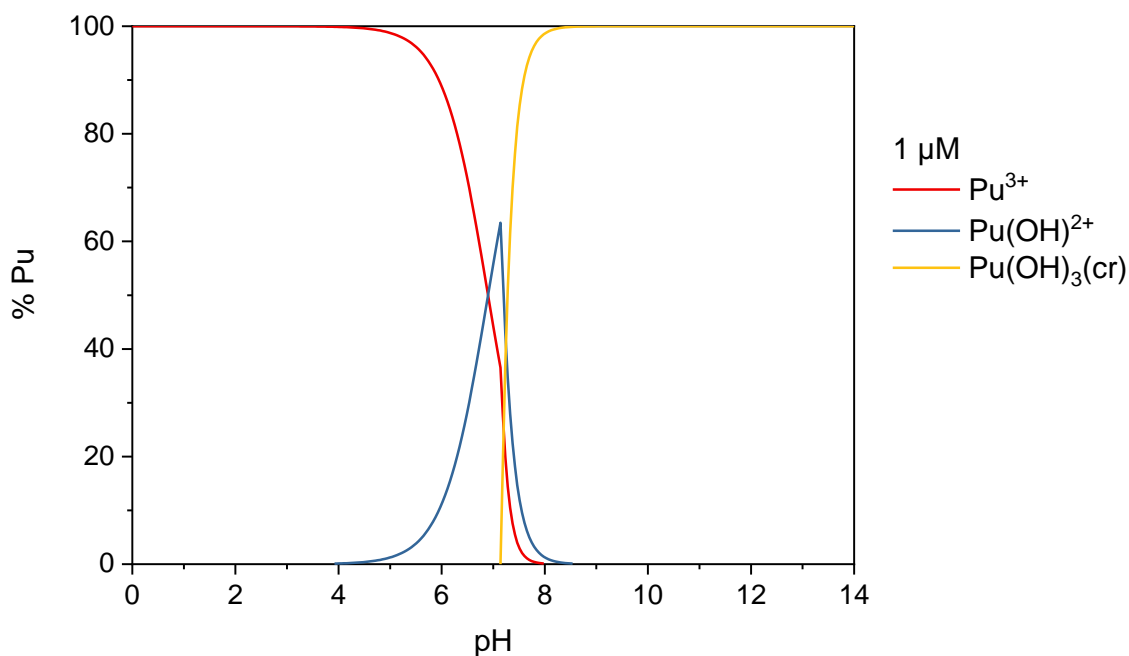
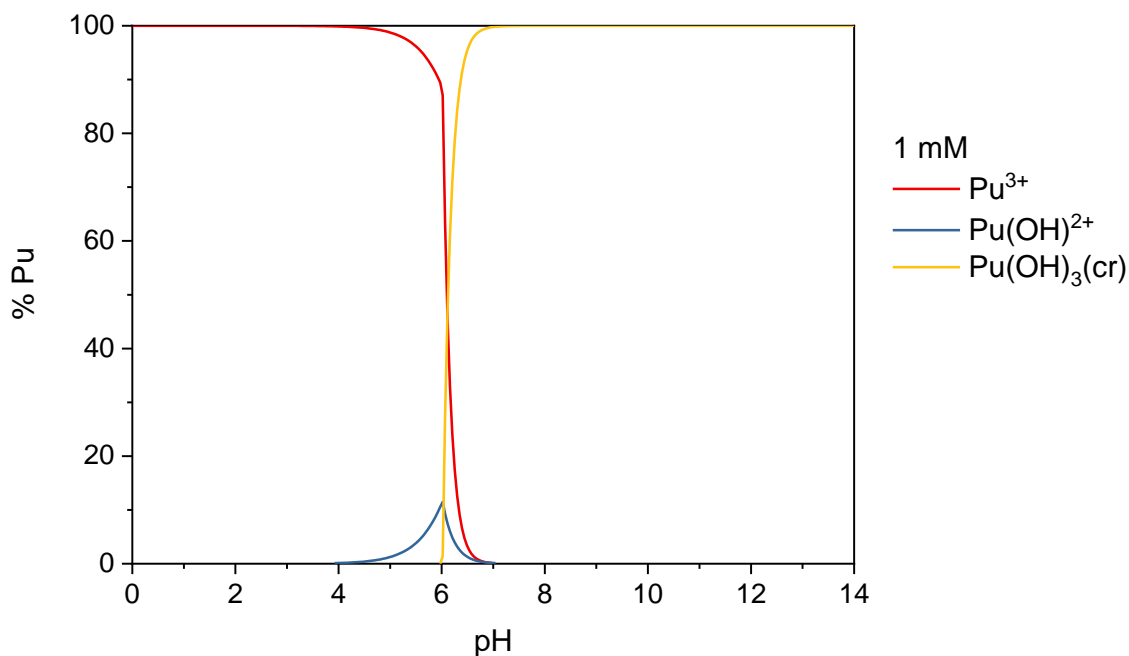
P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 396–397.

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

These diagrams have been computed at two Pu(III) 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

# Plutonium(IV)

Equilibrium reactions	lgK at infinite dilution and $T = 298\text{ K}$			
	Baes and Mesmer, 1976	NIST46	Brown and Ekberg, 2016	Grenthe et al., 2020
$\text{Pu}^{4+} + \text{H}_2\text{O} \rightleftharpoons \text{Pu}(\text{OH})^{3+} + \text{H}^+$	-0.5	-0.5	$-0.7 \pm 0.1$	$0.6 \pm 0.2$
$\text{Pu}^{4+} + 2 \text{H}_2\text{O} \rightleftharpoons \text{Pu}(\text{OH})_2^{2+} + 2 \text{H}^+$	(-2.3)			$0.6 \pm 0.3$
$\text{Pu}^{4+} + 3 \text{H}_2\text{O} \rightleftharpoons \text{Pu}(\text{OH})_3^+ + 3 \text{H}^+$	(-5.3)			$-2.3 \pm 0.4$
$\text{Pu}^{4+} + 4 \text{H}_2\text{O} \rightleftharpoons \text{Pu}(\text{OH})_4 + 4 \text{H}^+$	-9.5		$-12.5 \pm 0.7$	$-8.5 \pm 0.5$
$\text{Pu}^{4+} + 4 \text{OH}^- \rightleftharpoons \text{PuO}_2(\text{am, hyd}) + 2 \text{H}_2\text{O}$	49.5		$47.9 \pm 0.4$ (0w) $53.8 \pm 0.5$ (1w)	$58.3 \pm 0.5$

C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, pp. 187–189.

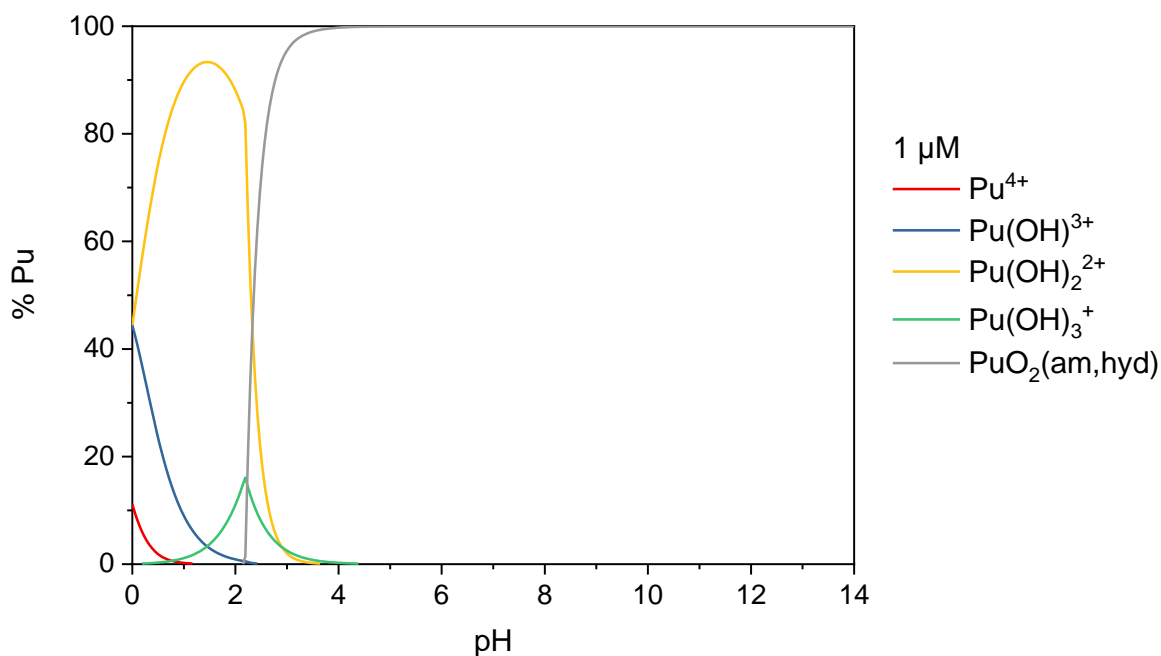
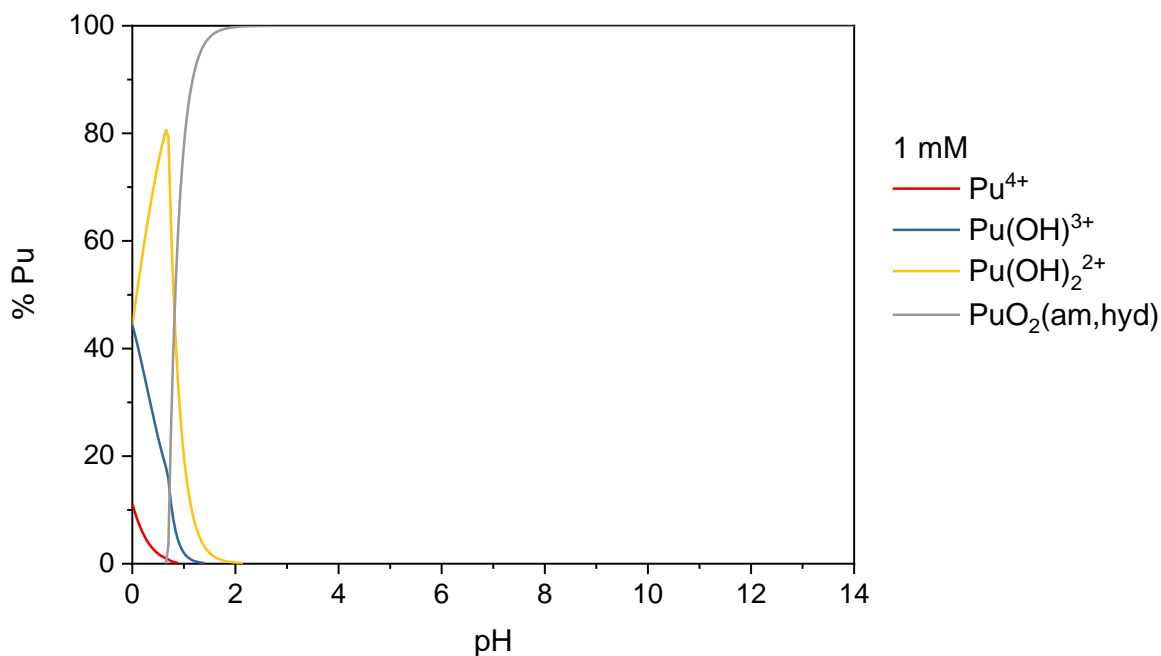
P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 397–401.

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

These diagrams have been computed at two Pu(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

# Plutonium(V)

Equilibrium reactions	lgK at infinite dilution and $T = 298\text{ K}$			
	Baes and Mesmer, 1976	NIST46	Brown and Ekberg, 2016	Grenthe et al., 2020
$\text{PuO}_2^+ + \text{H}_2\text{O} \rightleftharpoons \text{PuO}_2(\text{OH}) + \text{H}^+$	-9.7	-9.7		$\leq -9.73$
$\text{PuO}_2^+ + \text{H}_2\text{O} \rightleftharpoons \text{PuO}_2(\text{OH})(\text{am}) + \text{H}^+$	$\geq -5.4$	-5.4	$-5.0 \pm 0.3$	$-5.0 \pm 0.5$

C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, pp. 189–190.

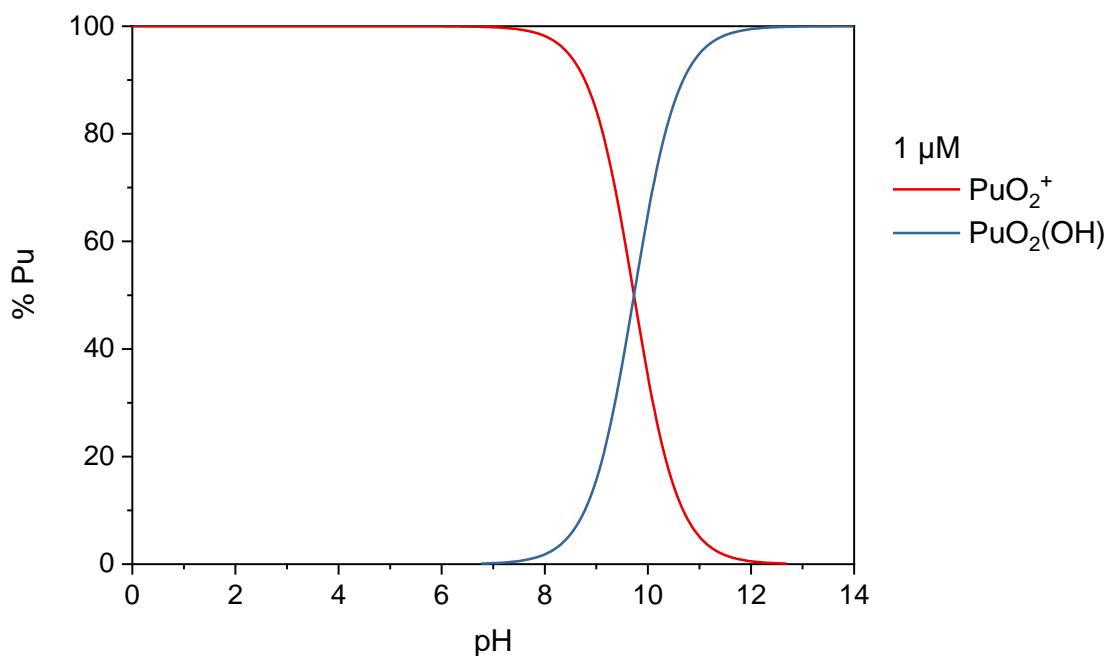
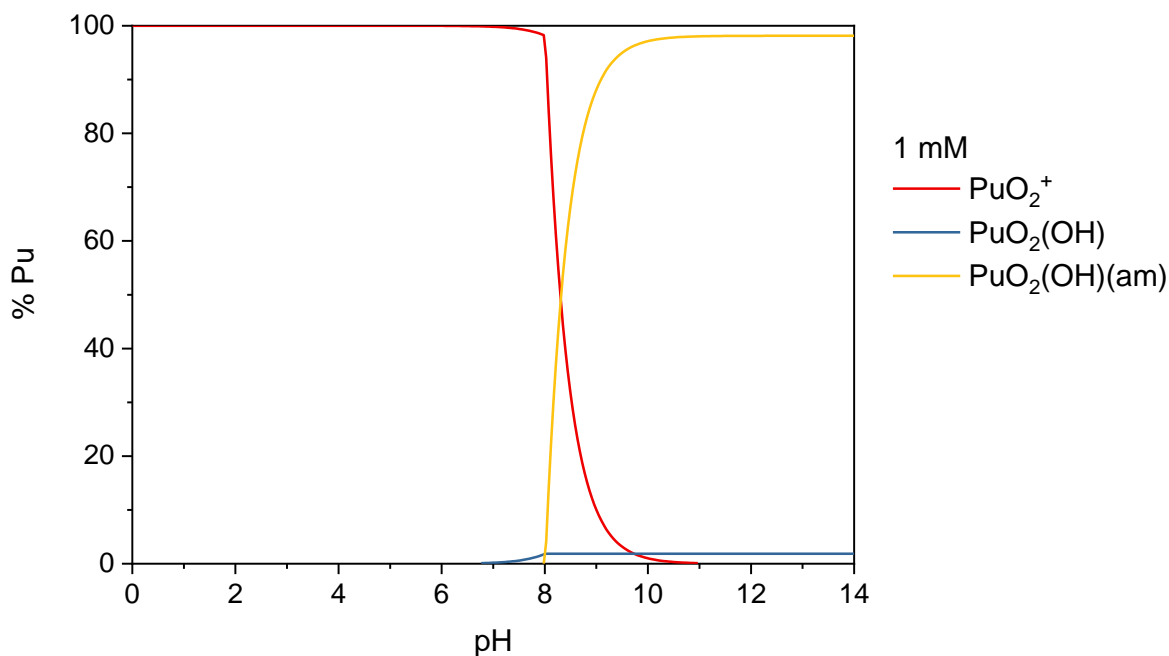
P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 401–403.

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

These diagrams have been computed at two Pu(V) 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

# Plutonium(VI)

Equilibrium reactions	lgK at infinite dilution and $T = 298\text{ K}$			
	Baes and Mesmer, 1976	NIST46	Brown and Ekberg, 2016	Grenthe et al., 2020
$\text{PuO}_2^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{PuO}_2(\text{OH})^+ + \text{H}^+$	-5.6	-5.6	$-5.36 \pm 0.09$	$-5.5 \pm 0.5$
$\text{PuO}_2^{2+} + 2 \text{H}_2\text{O} \rightleftharpoons \text{PuO}_2(\text{OH})_2 + 2 \text{H}^+$			$-12.9 \pm 0.2$	$-13 \pm 1$
$\text{PuO}_2^{2+} + 3 \text{H}_2\text{O} \rightleftharpoons \text{PuO}_2(\text{OH})_3^- + 3 \text{H}^+$				$-24 \pm 1$
$2 \text{PuO}_2^{2+} + 2 \text{H}_2\text{O} \rightleftharpoons (\text{PuO}_2)_2(\text{OH})_2^{2+} + 2 \text{H}^+$	-8.36	-8.36	$-7.8 \pm 0.5$	$-7 \pm 1$
$3 \text{PuO}_2^{2+} + 5 \text{H}_2\text{O} \rightleftharpoons (\text{PuO}_2)_3(\text{OH})_5^+ + 5 \text{H}^+$	-21.65	-21.65		
$\text{PuO}_2^{2+} + 2 \text{OH}^- \rightleftharpoons \text{PuO}_2(\text{OH})_2(\text{am, hyd})$				$22.8 \pm 0.6$

C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, pp. 190–191.

P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 403–405.

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.

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# Distribution diagrams

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

