

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

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 µM =  $1 \times 10^{-6}$  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).

