



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

## Neodymium

| Equilibrium reactions   | $\lg K$ at infinite dilution and $T = 298 \text{ K}$ |             |                             |                           |
|---|--|-------------|-----------------------------|---------------------------|
|   | Baes and<br>Mesmer, 1976                             | NIST46      | Neck et al.,<br>2009        | Brown and<br>Ekberg, 2016 |
| $Nd^{3+} + H_2O \rightleftharpoons Nd(OH)^{2+} + H^+$   | -8.0   | -8.0        | -7.4 ± 0.4                  | -8.13 ± 0.05              |
| $Nd^{3+} + 2 H_2O \rightleftharpoons Nd(OH)_2^+ + 2 H^+$  | (-16.9)  |             | -15.7 ± 0.7                 |                           |
| $Nd^{3+} + 3 H_2O \rightleftharpoons Nd(OH)_{3(aq)} + 3 H^+$  | (-26.5)  |             | -26.2 ± 0.5                 |                           |
| $Nd^{3+} + 4 H_2O \rightleftharpoons Nd(OH)_4^- + 4 H^+$  | (-37.1)  | -37.4       | -40.7 ± 0.7                 |                           |
| $2 \text{ Nd}^{3+} + 2 \text{ H}_2\text{O} \rightleftharpoons \text{Nd}_2(\text{OH})_2^{4+} + 2 \text{ H}^+$                    | -13.86   | -13.9       |                             | -15.56 ± 0.20             |
| 3 Nd <sup>3+</sup> + 5 H <sub>2</sub> O $\rightleftharpoons$ Nd <sub>3</sub> (OH) <sub>5</sub> <sup>4+</sup> + 5 H <sup>+</sup> | <-28.5   |             |                             | -34.2 ± 0.3               |
| $Nd(OH)_3(s) + 3 H^+ \rightleftharpoons Nd^{3+} + 3 H_2O$   | 18.6   |             | 17.2 ± 0.4                  | 17.89 ± 0.09              |
| $Nd(OH)_3(s) \rightleftharpoons Nd^{3+} + 3 OH^-$   |  | -23.2 ± 0.9 | -21.5 (act)<br>-23.1(inact) |                           |

C.F. Baes and R.E. Mesmer, The Hydrolysis of Cations. Wiley, New York, 1976, p. 137.

P.L. Brown and C. Ekberg, Hydrolysis of Metal Ions. Wiley, 2016, pp. 135-145.

V. Neck, M. Altmaier, T. Rabung, J. Lützenkirchen and T. Fanghänel, Thermodynamics of trivalent actinides and neodymium in NaCl, MgCl<sub>2</sub>, and CaCl<sub>2</sub> solutions: Solubility, hydrolysis, and ternary Ca-M(III)-OH complexes. Pure Appl. Chem., 81, 1555–1568 (2009).

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 Nd concentrations (1 mM =  $1x10^{-3}$  mol L<sup>-1</sup> and 1  $\mu$ M =  $1x10^{-6}$  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).



