Accessory publication

Palladium(II) sequestration by phytate in aqueous solution – speciation analysis and ionic medium effects

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Table A1. Phytate protonation constants in NaCl$_{aq}$[36] and in NaNO$_{3aq}$[35] at $I = 0.1$ mol L^{-1} and $t = 25°$C

$\log\beta_r^H$ refer to equilibrium: $Phy^{12-} + r\ H^+ = H_rPhy^{(12-r)-}$; $\log K_r^H$ in parenthesis refer to equilibrium: $H^+ + H_{r-1}Phy^{(12-r+1)-} = H_rPhy^{(12-r)-}$

Medium	$\log\beta_1^H$	$\log\beta_2^H$	$\log\beta_3^H$	$\log\beta_4^H$	$\log\beta_5^H$	$\log\beta_6^H$	$\log\beta_7^H$
NaCl$_{aq}$	9.58	19.42	28.92	37.06	43.56	48.81	51.69
		(9.84)	(9.50)	(8.14)	(6.50)	(5.25)	(2.88)
NaNO$_{3aq}$	9.48	19.46	28.99	37.19	43.68	48.85	51.87
		(9.98)	(9.53)	(8.20)	(6.49)	(5.17)	(3.02)

Table A2. Literature values for palladium(II) hydrolysis in NaClO$_{4aq}$ at $t = 25°$C and different ionic strengths

$\log\beta_{10r}$ refer to equilibrium: $Pd^{2+} + r\ H_2O = Pd(OH)_r^{(2-r)} + r\ H^+$

I (mol L^{-1})	$\log\beta_{10-1}$	$\log\beta_{10-2}$	$\log\beta_{10-3}$	$\log\beta_{10-4}$	References
0[A]	~−1.3	~−1.85	–	–	[24]
0.05	−1.2	−2.2	–	–	[24]
0.1	−1.38	−2.36	–	–	[24]
0.1[B]	−2.08	−3.99	−15.92	−28.7	[25]
0.1	–	−3.76	–	–	[19]
0.18	−1.76	−2.82	–	–	[24]
0.5	−1.77	−4.24	–	–	[19]
0.5–1[C]	−5.65	−12.2	−19.85	−28.5	[18]
variable	–	~−8.7	~−20.5	–	[18][D]
1	−3.0	–	–	–	[28]
1	–	−4.1	−15.05	–	[19]

[A]Values extrapolated by a Debye–Hückel type equation.

[B]Values at $t = 17°$C.

[C]Only one value given by the authors in this ionic strength range.

[D]Literature values reported by authors.

Table A3. Literature values for palladium(II) hydrolysis and chloride complexes chloride aqueous media, at different temperatures and ionic strengths

$\log \beta_{pqr}$ refer to equilibrium: p Pd^{2+} + q Cl^- + r H_2O = $Pd_pCl_q(OH)_r^{(2p-q-r)}$ + r H^+; data in parenthesis refer to

$\log K_{PdClq}$ for the stepwise equilibrium: $PdCl_{(q-1)}^{(2-q+1)}$ + Cl^- = $PdCl_q^{(2-q)}$. ?, not specified

Medium	I (mol L^{-1})	t (°C)	$\log \beta_{110}$	$\log \beta_{120}$	$\log \beta_{130}$	$\log \beta_{140}$	$\log \beta_{13-1}$	$\log \beta_{12-2}$	$\log \beta_{10-1}$	References
	0	21	6.2	10.9	13.4	16	–	–	–	[14]
	0	25	–	–	–	11.29	6.29	–	–	[19]
	0	25	–	–	–	–	2.04 [A]	–	–	[20]
	0	20	5.080	8.555	10.655	11.557	–	–	–	[21]
	0	25	5.08	8.88	11.30	12.18	–	–	–	[30]
KCl	0.1	25	–	–	–	11.81	6.43	–	–	[19]
ClO$_4$ / Cl$^-$	0.1	?	3.48	6.27	8.62	9.72	–	–	–	[19] [B]
NaClO$_4$ / Cl$^-$	0.1	25	6.0	10.6	13.1	–	–	–	–	[30]
NaCl	0.105	25	–	–	–	–	3.09 [A]	–	–	[29]
NaCl	0.305	25	–	–	–	–	2.93 [A]	–	–	[29]
NaCl	0.5	25	–	–	–	–	–	–	–9.23 [C]	[16] [D]
KCl	0.5	25	–	–	–	11.83	5.64	–	–	[19]
NaCl	0.5	25	–	–	–	–	2.85 [A]	–	–	[20]
NaCl	0.505	25	–	–	–	–	2.86 [A]	–	–	[29]
Cl$^-$ / ClO$_4^-$	0.5–1 [E]	25	4.21	7.5	9.88	11.32	2.37 [F]	–7.5 [F]	–	[18] [G]
NaCl	0.6 [H]	25	–	–	–	–	~2.42 [I]	–7.82 [I]	–	[22]
NaCl	0.705	25	–	–	–	–	2.82 [A]	–	–	[29]
?	0.8	20	4.34	7.88	10.56	12.24	–	–	–	[23] [B]
NaClO$_4$ / NaCl	0.86	25	3.98	7.22	9.52	11.52	–	–	–	[17] [B]
HClO$_4$ / NaCl	1	25	3.88	6.91	9.09	10.43	–	–	–	[23]
HClO$_4$ / HCl	1	25	4.47	7.76	10.17	11.54	–	–	–	[15]
NaCl	1	25	–	–	–	–	–	–	–9.30 [C]	[16] [D]
NaCl	1.5	25	–	–	–	–	–	–	–9.35 [C]	[16] [D]
KCl	1	25	–	–	–	11.78	4.48	–	–	[19]
NaClO$_4$ / Cl$^-$	1	?	–	–	–	(1.27)	–	–	–	[30]
NaClO$_4$ / Cl$^-$	1	25	–	–	–	12.15	–	–	–	[30]
NaCl	1.005	25	–	–	–	–	2.82 [A]	–	–	[29]
NaCl	2	25	–	–	–	–	–	–	–9.39 [C]	[16] [D]
NaCl	2.5	25	–	–	–	–	–	–	–9.45 [C]	[16] [D]
NaCl	3	25	–	–	–	–	–	–	–9.61 [C]	[16] [D]
H$_2$SO$_4$ / Cl$^-$	3	25	–	–	(1.76)	(2.35)	–	–	–	[30]

[A]$\log \beta_{140}$ from ref. [19] was used in calculations.

[B]Literature values reported by authors.

[C]Conditional formation constants with respect to palladium(II)–chloride species.

[D]Further species reported by authors: $-30.51 \leq \log \beta_{40-4} \leq -28.81$ in the range $0.5 \leq I$ (mol L^{-1}) ≤ 3.0.

[E]Only one value given by the authors in this ionic strength range.

[F]At $I = 0.7$ mol L^{-1}.

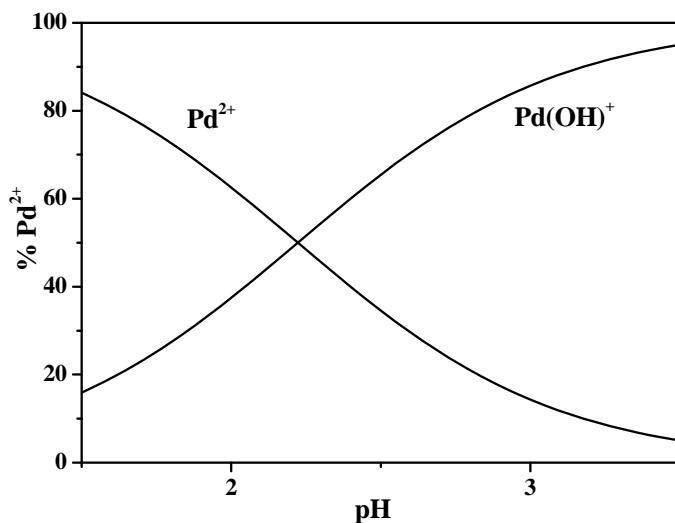[G]Other species reported by authors as recommended data: $\log \beta_{11-3} = -17.65$.

[H]In mol kg^{-1}.

[I]$\log \beta_{pq0}$ from ref. [18] were used in calculations.

Table A4. Literature values for palladium(II) hydrolysis and nitrate complexes in HNO_{3aq} / $NaNO_{3aq}$ or HNO_{3aq} / $NaClO_{4aq}$ at different temperatures and ionic strengths

$\log\beta_{pqr}$ refer to equilibrium: $p\ Pd^{2+} + q\ NO_3^- + r\ H_2O = Pd_p(NO_3)_q(OH)_r^{(2p-q-r)} + r\ H^+$; ?, not specified

I (mol L^{-1})	t (°C)	$\log\beta_{110}$	$\log\beta_{120}$	$\log\beta_{130}$	$\log\beta_{140}$	$\log\beta_{11-1}$	References
≤5	?	0.08	–	–	–	–	[26]
5.18	25	0.17	–0.76	–	–	–0.64	[27]
?	?	1.14	0.3	0.78	–	–	[31]
?	?	0.51	0.32	–0.65	–2.40	–	[31]
4	?	0.2	–	–	–	–	[32]

Fig. A1. Distribution diagram of palladium hydrolytic species *v.* pH, at $I = 0.1$ mol L^{-1} in $NaNO_{3aq}$ at $t = 25$°C, obtained considering the conditional hydrolysis constants of Table 2. Experimental conditions: $C_{Pd} = 1$ mmol L^{-1}.