

Supplementary material

Table S1 Thermodynamic formation constants of the aqueous species used in calculation

Reaction	logK	Source of logK
$\text{H}_2\text{O} \rightleftharpoons \text{OH}^- + \text{H}^+$	-13.997	NIST46.4
$\text{H}^+ + \text{CO}_3^{2-} \rightleftharpoons \text{HCO}_3^-$	10.329	PlumBus82
$2\text{H}^+ + \text{CO}_3^{2-} \rightleftharpoons \text{H}_2\text{CO}_3$	16.681	NIST46.7
$\text{H}^+ + \text{SO}_4^{2-} \rightleftharpoons \text{HSO}_4^-$	1.99	NIST46.7
$\text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{HPO}_4^{2-}$	12.375	NIST46.7
$2\text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{H}_2\text{PO}_4^-$	19.573	NIST46.7
$3\text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{H}_3\text{PO}_4$	21.721	NIST46.7
$\text{H}^+ + \text{glycine}^- \rightleftharpoons \text{H}(\text{glycine})$	9.778	NIST46.6
$2\text{H}^+ + \text{glycine}^- \rightleftharpoons \text{H}_2(\text{glycine})^+$	12.128	NIST46.6
$\text{Na}^+ + \text{OH}^- \rightleftharpoons \text{NaOH}$	0.1	NIST46.7
$\text{Na}^+ + \text{Cl}^- \rightleftharpoons \text{NaCl}$	-0.3	NIST46.7
$\text{Na}^+ + \text{CO}_3^{2-} \rightleftharpoons \text{NaCO}_3^-$	1.27	NIST46.7
$\text{Na}^+ + \text{H}^+ + \text{CO}_3^{2-} \rightleftharpoons \text{NaHCO}_3$	10.079	NIST46.7
$\text{Na}^+ + \text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{NaHPO}_4^-$	13.445	NIST46.7
$\text{Na}^+ + \text{PO}_4^{3-} + 2\text{H}^+ \rightleftharpoons \text{NaH}_2\text{PO}_4$	19.873	NIST46.7
$\text{Na}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{NaPO}_4^{2-}$	1.43	NIST46.7
$2\text{Na}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{Na}_2\text{PO}_4^-$	1.16	NIST46.7
$2\text{Na}^+ + \text{PO}_4^{3-} + \text{H}^+ \rightleftharpoons \text{Na}_2\text{HPO}_4$	13.32	NIST46.7
$\text{K}^+ + \text{H}_2\text{O} \rightleftharpoons \text{KOH} + \text{H}^+$	-13.757	NIST46.7
$\text{K}^+ + \text{Cl}^- \rightleftharpoons \text{KCl}$	-0.3	NIST46.7
$\text{K}^+ + \text{SO}_4^{2-} \rightleftharpoons \text{KSO}_4^-$	0.85	NIST46.7
$\text{K}^+ + \text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{KHPO}_4^-$	13.255	NIST46.7
$\text{K}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{KPO}_4^{2-}$	1.43	NIST46.7
$2\text{K}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{K}_2\text{PO}_4^-$	0.83	NIST46.7
$\text{K}^+ + \text{PO}_4^{3-} + 2\text{H}^+ \rightleftharpoons \text{KH}_2\text{PO}_4$	19.873	NIST46.7
$2\text{K}^+ + \text{PO}_4^{3-} + \text{H}^+ \rightleftharpoons \text{K}_2\text{HPO}_4$	13.44	NIST46.7
$\text{Mg}^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{MgOH}^+ + \text{H}^+$	-11.397	NIST46.7
$\text{Mg}^{2+} + \text{Cl}^- \rightleftharpoons \text{MgCl}^+$	0.6	NIST46.7
$\text{Mg}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{MgCO}_3$	2.92	NIST46.7
$\text{Mg}^{2+} + \text{H}^+ + \text{CO}_3^{2-} \rightleftharpoons \text{MgHCO}_3^+$	11.339	NIST46.7
$\text{Mg}^{2+} + \text{SO}_4^{2-} \rightleftharpoons \text{MgSO}_4$	2.26	NIST46.7

$\text{Mg}^{2+} + \text{PO}_4^{3-} \rightleftharpoons \text{MgPO}_4^-$	4.654	Turner et al.1981
$\text{Mg}^{2+} + \text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{MgHPO}_4$	15.175	NIST46.7
$\text{Mg}^{2+} + 2\text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{MgH}_2\text{PO}_4^+$	21.2561	NIST46.7
$\text{Mg}^{2+} + \text{glycine}^- \rightleftharpoons \text{Mg}(\text{glycine})^+$	2.08	NIST46.6
$\text{Ca}^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{CaOH}^+ + \text{H}^+$	-12.697	NIST46.7
$\text{Ca}^{2+} + \text{Cl}^- \rightleftharpoons \text{CaCl}^+$	0.4	NIST46.7
$\text{Ca}^{2+} + \text{H}^+ + \text{CO}_3^{2-} \rightleftharpoons \text{CaHCO}_3^+$	11.599	NIST46.3
$\text{Ca}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{CaCO}_3$	3.2	NIST46.3
$\text{Ca}^{2+} + \text{SO}_4^{2-} \rightleftharpoons \text{CaSO}_4$	2.36	NIST46.7
$\text{Ca}^{2+} + \text{PO}_4^{3-} \rightleftharpoons \text{CaPO}_4^-$	6.46	Turner et al.1981
$\text{Ca}^{2+} + \text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{CaHPO}_4$	15.035	NIST46.7
$\text{Ca}^{2+} + 2\text{H}^+ + \text{PO}_4^{3-} \rightleftharpoons \text{CaH}_2\text{PO}_4^+$	20.923	NIST46.7
$\text{Ca}^{2+} + \text{glycine}^- \rightleftharpoons \text{Ca}(\text{glycine})^+$	1.39	NIST46.6
$\text{Zn}^{2+} + \text{H}_2\text{O} \rightleftharpoons \text{ZnOH}^+ + \text{H}^+$	-8.997	NIST46.7
$\text{Zn}^{2+} + 2\text{H}_2\text{O} \rightleftharpoons \text{Zn}(\text{OH})_2 + 2\text{H}^+$	-16.894	NIST46.7
$\text{Zn}^{2+} + 3\text{H}_2\text{O} \rightleftharpoons \text{Zn}(\text{OH})_3^- + 3\text{H}^+$	-28.391	NIST46.7
$\text{Zn}^{2+} + 4\text{H}_2\text{O} \rightleftharpoons \text{Zn}(\text{OH})_4^{2-} + 4\text{H}^+$	-41.188	NIST46.7
$2\text{Zn}^{2+} + \text{OH}^- \rightleftharpoons \text{Zn}_2\text{OH}^{3+}$	-8.997	NIST46.7
$\text{Zn}^{2+} + \text{Cl}^- \rightleftharpoons \text{ZnCl}^+$	0.46	NIST46.7
$\text{Zn}^{2+} + 2\text{Cl}^- \rightleftharpoons \text{ZnCl}_2$	0.6	NIST46.3
$\text{Zn}^{2+} + 3\text{Cl}^- \rightleftharpoons \text{ZnCl}_3^-$	0.510	Turner et al.1981
$\text{Zn}^{2+} + 4\text{Cl}^- \rightleftharpoons \text{ZnCl}_4^{2-}$	0.2	Turner et al.1981
$\text{Zn}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{ZnCO}_3$	4.76	NIST46.7
$\text{Zn}^{2+} + \text{H}^+ + \text{CO}_3^{2-} \rightleftharpoons \text{ZnHCO}_3^+$	11.829	NIST46.7
$\text{Zn}^{2+} + 2\text{CO}_3^{2-} \rightleftharpoons \text{Zn}(\text{CO}_3)_2^{2-}$	7.3	NIST46.7
$\text{Zn}^{2+} + \text{SO}_4^{2-} \rightleftharpoons \text{ZnSO}_4$	2.34	NIST46.3
$\text{Zn}^{2+} + \text{PO}_4^{3-} + \text{H}^+ \rightleftharpoons \text{ZnHPO}_4$	15.689	NIST46.8
$\text{Zn}^{2+} + \text{PO}_4^{3-} + 2\text{H}^+ \rightleftharpoons \text{ZnH}_2\text{PO}_4^+$	19.403	NIST46.8
$\text{Zn}^{2+} + \text{glycine}^- \rightleftharpoons \text{Zn}(\text{glycine})^+$	5.38	NIST46.6

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Table S2 Thermodynamic formation constants of the solids used in calculation

Solid phase	Reaction	log K	Source of log K
Halite	$\text{NaCl} = \text{Na}^+ + \text{Cl}^-$	1.550	NIST 46.8
Natron	$\text{Na}_2\text{CO}_3 \cdot 10\text{H}_2\text{O} = 2\text{Na}^+ + \text{CO}_3^{2-} + 10\text{H}_2\text{O}$	-1.311	MTQ 3.11
Nahcolite	$\text{NaHCO}_3 = \text{Na}^+ + \text{HCO}_3^-$	-0.548	Wateq 4f
Trona	$\text{NaHCO}_3 \cdot \text{Na}_2\text{CO}_3 \cdot 2\text{H}_2\text{O} = 2\text{H}_2\text{O} + 3\text{Na}^+ + \text{CO}_3^{2-} + \text{HCO}_3^-$	-0.795	Wateq 4f
Mirabilite	$\text{Na}_2\text{SO}_4 \cdot 10\text{H}_2\text{O} = 2\text{Na}^+ + \text{SO}_4^{2-} + 10\text{H}_2\text{O}$	-1.114	MTQ 3.11
Thenardite	$\text{Na}_2\text{SO}_4 = 2\text{Na}^+ + \text{SO}_4^{2-}$	0.3217	NIST 13.1
Mg(OH) ₂ (active)	$\text{Mg(OH)}_2 + 2\text{H}^+ = \text{Mg}^{2+} + 2\text{H}_2\text{O}$	18.794	NIST 46.7
Artinite	$\text{MgCO}_3 \cdot \text{Mg(OH)}_2 \cdot 3\text{H}_2\text{O} + 2\text{H}^+ = 2\text{Mg}^{2+} + \text{CO}_3^{2-} + 5\text{H}_2\text{O}$	9.6	MTQ 3.11
Hydromagnesite	$\text{Mg}_5(\text{CO}_3)_4(\text{OH})_2 \cdot 4\text{H}_2\text{O} + 2\text{H}^+ = 5\text{Mg}^{2+} + 4\text{CO}_3^{2-} + 6\text{H}_2\text{O}$	-8.766	MTQ 3.11
Magnesite	$\text{MgCO}_3 = \text{Mg}^{2+} + \text{CO}_3^{2-}$	-7.46	NIST 46.7
Nesquehonite	$\text{MgCO}_3 \cdot 3\text{H}_2\text{O} = \text{Mg}^{2+} + \text{CO}_3^{2-} + 3\text{H}_2\text{O}$	-4.67	NIST 46.7
Huntite	$\text{CaMg}_3(\text{CO}_3)_4 = 3\text{Mg}^{2+} + \text{Ca}^{2+} + 4\text{CO}_3^{2-}$	-29.968	MTQ 3.11
Epsomite	$\text{MgSO}_4 \cdot 7\text{H}_2\text{O} = \text{Mg}^{2+} + \text{SO}_4^{2-} + 7\text{H}_2\text{O}$	-2.1265	NIST 2.1.1
Mg ₃ (PO ₄) ₂	$\text{Mg}_3(\text{PO}_4)_2 = 3\text{Mg}^{2+} + 2\text{PO}_4^{3-}$	-23.28	NIST 46.7
MgHPO ₄ ·3H ₂ O	$\text{MgHPO}_4 \cdot 3\text{H}_2\text{O} = \text{Mg}^{2+} + \text{H}^+ + \text{PO}_4^{3-} + 3\text{H}_2\text{O}$	-18.175	NIST 46.7
Portlandite	$\text{Ca(OH)}_2 + 2\text{H}^+ = \text{Ca}^{2+} + 2\text{H}_2\text{O}$	22.804	NIST 46.7
Aragonite	$\text{CaCO}_3 = \text{Ca}^{2+} + \text{CO}_3^{2-}$	-8.3	PlumBus82
Gypsum	$\text{CaSO}_4 \cdot 2\text{H}_2\text{O} = \text{Ca}^{2+} + \text{SO}_4^{2-} + 2\text{H}_2\text{O}$	-4.61	PlumBus82
Hydroxylapatite	$\text{Ca}_5(\text{PO}_4)_3(\text{OH}) = 5\text{Ca}^{2+} + 3\text{PO}_4^{3-} + \text{OH}^-$	-58.4	Tung 88
CaHPO ₄ ·2H ₂ O	$\text{CaHPO}_4 \cdot 2\text{H}_2\text{O} = \text{Ca}^{2+} + \text{H}^+ + \text{PO}_4^{3-} + 2\text{H}_2\text{O}$	-18.995	NIST 46.4
Ca ₄ H(PO ₄) ₃ ·2.5H ₂ O	$\text{Ca}_4\text{H}(\text{PO}_4)_3 \cdot 2.5\text{H}_2\text{O} = 4\text{Ca}^{2+} + \text{H}^+ + 3\text{PO}_4^{3-} + 2.5\text{H}_2\text{O}$	-48.30	McD 77
Ca ₃ (PO ₄) ₂ (am)	$\text{Ca}_3(\text{PO}_4)_2 = 3\text{Ca}^{2+} + 2\text{PO}_4^{3-}$	-25.8	CHRIS 90
Whitlockite	$\text{Ca}_9\text{Mg}(\text{HPO}_4)(\text{PO}_4)_6 = 9\text{Ca}^{2+} + \text{Mg}^{2+} + \text{H}^+ + 7\text{PO}_4^{3-}$	-106.34	Hamad and Heughebaert, 86
Zn(OH) ₂ (am)	$\text{Zn(OH)}_2 + 2\text{H}^+ = \text{Zn}^{2+} + 2\text{H}_2\text{O}$	12.474	NIST 46.4
Zn(OH) ₂ (epsilon)	$\text{Zn(OH)}_2 + 2\text{H}^+ = \text{Zn}^{2+} + 2\text{H}_2\text{O}$	11.534	NIST 46.4
Zn ₂ (OH) ₃ Cl	$\text{Zn}_2(\text{OH})_3\text{Cl} + 3\text{H}^+ = 2\text{Zn}^{2+} + 3\text{H}_2\text{O} + \text{Cl}^-$	15.191	NIST 46.4
Zn ₅ (OH) ₈ Cl ₂	$\text{Zn}_5(\text{OH})_8\text{Cl}_2 + 8\text{H}^+ = 5\text{Zn}^{2+} + 8\text{H}_2\text{O} + 2\text{Cl}^-$	38.5	MTQ 3.11

ZnCl ₂	$\text{ZnCl}_2 = \text{Zn}^{2+} + 2\text{Cl}^-$	7.05	NIST 2.1.1
Zn ₂ (OH) ₂ SO ₄	$\text{Zn}_2(\text{OH})_2\text{SO}_4 + 2\text{H}^+ = 2\text{Zn}^{2+} + 2\text{H}_2\text{O} + \text{SO}_4^{2-}$	7.5	MTQ 3.11
Zn ₄ (OH) ₆ SO ₄	$\text{Zn}_4(\text{OH})_6\text{SO}_4 + 6\text{H}^+ = 4\text{Zn}^{2+} + 6\text{H}_2\text{O} + \text{SO}_4^{2-}$	28.4	MTQ 3.11
Zn ₃ O(SO ₄) ₂	$\text{Zn}_3\text{O}(\text{SO}_4)_2 + 2\text{H}^+ = 3\text{Zn}^{2+} + 2\text{SO}_4^{2-} + \text{H}_2\text{O}$	18.9135	NIST 2.1.1
Zincosite	$\text{ZnSO}_4 = \text{Zn}^{2+} + \text{SO}_4^{2-}$	3.9297	NIST 13.1
ZnSO ₄ ·1H ₂ O	$\text{ZnSO}_4 \cdot 1\text{H}_2\text{O} = \text{Zn}^{2+} + \text{SO}_4^{2-} + \text{H}_2\text{O}$	-0.638	NIST 2.1.1
Bianchite	$\text{ZnSO}_4 \cdot 6\text{H}_2\text{O} = \text{Zn}^{2+} + \text{SO}_4^{2-} + 6\text{H}_2\text{O}$	-1.765	MTQ 3.11
Goslarite	$\text{ZnSO}_4 \cdot 7\text{H}_2\text{O} = \text{Zn}^{2+} + \text{SO}_4^{2-} + 7\text{H}_2\text{O}$	-2.0112	NIST 2.1.1
Zn ₃ (PO ₄) ₂ ·4H ₂ O	$\text{Zn}_3(\text{PO}_4)_2 \cdot 4\text{H}_2\text{O} = 3\text{Zn}^{2+} + 2\text{PO}_4^{3-} + 4\text{H}_2\text{O}$	-35.42	NIST 46.7

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