GEOCHEMICAL BEHAVIOR OF RARE EARTH ELEMENTS IN ACID DRAINAGES: MODELING ACHIEVEMENTS AND LIMITATIONS

Alba Lozano[a], Carlos Ayora[a], Francisco Macías[a,b], Rafael León[b], María José Gimeno[c], Luis Auqué[c]

[a] Institute of Environmental Assessment and Water Research, (IDAEA-CSIC), Jordi Girona 18-26, 08034 Barcelona, Spain

[b]Department of Earth Sciences & Research Centre on Natural Resources, Health and the Environment (RENSMA), Faculty of Experimental Sciences, University of Huelva, Campus “El Carmen”, E-21071, Huelva, Spain

[c]Geochemical Modelling Group. Petrology and Geochemistry Area, Earth Science Department, University of Zaragoza, Spain C/ Pedro Cerbuna 12, 50009, Zaragoza

Corresponding author:

Alba Lozano (alba.lozano@idaea.csic.es)

Annex

Table S1. Aqueous speciation constants for Sc, Y and lanthanides (M) with different ligands (L). References: a: Klugness & Byrne, 2000 ; b: Lee & Byrne, 92; c: Luo & Byrne, 2004;d: Millero, 92; e: Luo & Millero, 2004; f: Schijf & Byrne, 2004; g: Luo & Byrne,2001; h: Wood and Samson, 2006 (for Sc speciation).

Reaction	$\log {}_L\beta_n$	Sc	Y	La	Ce	Pr	Nd	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Ref
$M^{+3} + H_2O = M(OH)^{+2}$ + I	$\log {}_{OH}\beta^*_1$	-4.31	-7.8	-8.81	-8.34	-8.32	-8.18	-7.84	-7.76	-7.83	-7.64	-7.59	-7.56	-7.52	-7.39	-7.45	-7.27	a
$M^{+3} + 2H_2O = M(OH)_2^{+}$ + 2	$\log {}_{OH}\beta^*_2$	-9.7	-16.4	-18.14	-17.6	-17.27	-17.04	-16.51	-16.37	-16.37	-16.18	-16.1	-16.07	-15.96	-15.88	-15.74	-15.67	b, h
$M^{+3} + 3H_2O = M(OH)_3$ + 3	$\log {}_{OH}\beta^*_3$	-16.1	-25.99	-27.9	-27.23	-26.63	-26.4	-25.91	-25.41	-25.28	-25.08	-24.83	-24.56	-24.35	-24.18	-23.85	-23.85	b, h
$M^{+3} + CO_3^{-2} = MCO_3^{+}$	$\log {}_{CO3}\beta_1$	-	7.48	6.73	7.06	7.23	7.28	7.46	7.48	7.39	7.46	7.56	7.55	7.61	7.68	7.81	7.75	c
$M^{+3} + HCO_3^{-} = MHCO_3^{+3}$	$\log {}_{HCO3}\beta_1$	-	2.32	2.34	2.31	2.25	2.28	2.34	2.47	2.36	2.46	2.5	2.46	2.49	2.52	2.53	2.49	c
$M^{+3} + 2CO_3^{-2} = M(CO3)_2^{-}$	$\log {}_{CO3}\beta_2$	-	12.63	11.3	11.76	12.08	12.17	12.53	12.63	12.48	12.78	12.91	13	13.12	13.27	13.3	13.37	c
$Ln^{+3} + NO_3^{-} = LnNO_3^{+2}$	$\log {}_{NO3}\beta_1$	-	-	0.58	0.69	0.69	0.79	0.78	0.83	0.47	0.51	0.15	0.25	0.15	0.2	0.25	0.56	d
$M^{+3} + F^{-} = MF^{+2}$	$\log {}_{F}\beta_1$	-	3.97	3.11	3.29	3.35	3.29	3.61	3.72	3.71	3.83	3.88	3.78	3.77	3.77	3.84	3.74	e
$M^{+3} + 2F^{-} = MF_2^{+}$	$\log {}_{F}\beta_2$	-	6.35	5.16	5.48	5.66	5.66	5.99	6.11	6.07	6.24	6.29	5.98	5.96	6.09	6.31	6.31	e
$Ln^{+3} + SO_4^{-2} = LnSO_4^{+}$	$\log {}_{so4}\beta_1$	4.18	3.5	3.61	3.61	3.62	3.6	3.63	3.64	3.61	3.59	3.57	3.54	3.51	3.48	3.46	3.44	f,h
$M^{+3} + Cl^{-} = MCl^{+2}$	$\log {}_{Cl}\beta_1$	-	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	0.65	g

Table S2. Equilibrium constants for the REE surface complexation reactions onto basaluminite (Lozano et al., 2019a).

Element	Surface Complex	Log K
Sc	$(XO)_2ScSO_4^{-}$	-5.19
	$XOSc(OH)_2$	-5.81
Y	$XOYSO_4$	-2.48
La	$XOLaSO_4$	-2.95
Ce	$XOCeSO_4$	-2.81
Pr	$XOPrSO_4$	-2.69
Nd	$XONdSO_4$	-2.60
Sm	$XOSmSO_4$	-2.48
Eu	$XOEuSO_4$	-2.50
Gd	$XOGdSO_4$	-2.50
Tb	$XOTbSO_4$	-2.48
Dy	$XODySO_4$	-2.37
Ho	$XOHoSO_4$	-2.40
Er	$XOErSO_4$	-2.40
Tm	$XOTmSO_4$	-2.27
Yb	$XOYbSO_4$	-2.13
Lu	$XOLuSO_4$	-2.19