

Yttrium speciation in subduction zone fluids from *ab initio* molecular dynamics simulations

Supporting Information

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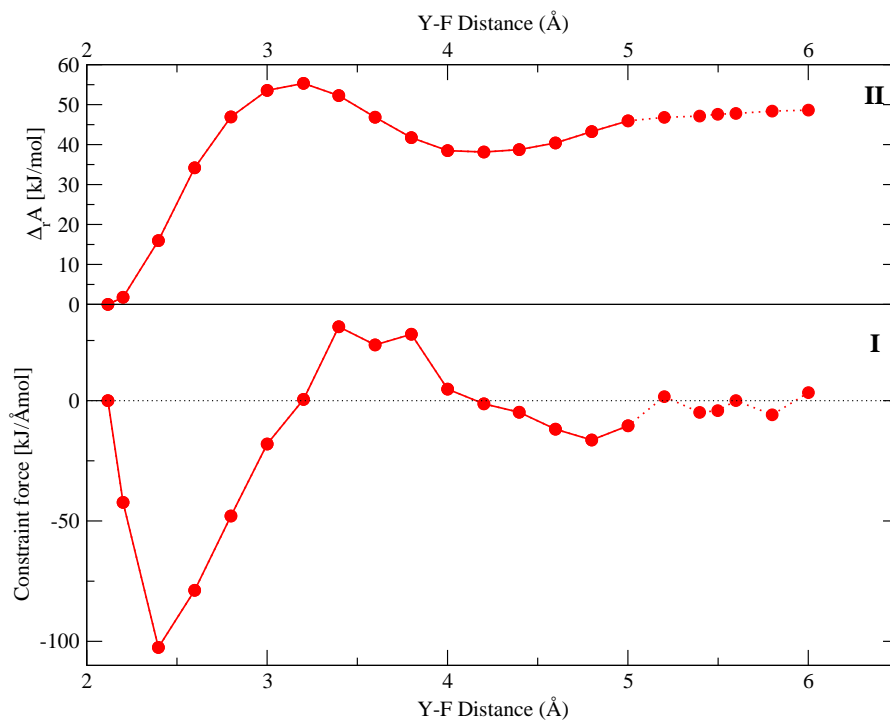


Figure S1: (I) potential of mean force of the dissociation reaction of YFOH^+ to YOH^{2+} at 4.5 GPa and 800 °C for a integration length of 5.0 Å and 6.0 Å, (II) resulting Helmholtz free energy along the integration pathway.

Table S1: Hydration number of halide ions for associated (Y)Cl and (Y)F complexes and dissociated halide ions (Cl^- and F^-). For the Y chloride complexes, only those are considered that persist for at least 10 ps in the AIMD simulations. Δ refers to the number of H_2O molecules that are released during association of the halide ion with Y.

run ID	initial	ρ ($\frac{\text{kg}}{\text{m}^3}$)	time (ps)	cell	(Y)Cl- H_2O	Cl^- - H_2O	Δ_{Cl}	(Y)F- H_2O	F^- - H_2O	Δ_{F}
#1	$[\text{YCl}(\text{H}_2\text{O})_5]^{2+}$	1072	25	A1	3	4	1	-	-	-
#2	$[\text{YCl}_2(\text{H}_2\text{O})_4]^+$	1072	23	A1	2	4	2	-	-	-
#3	$[\text{YCl}_3(\text{H}_2\text{O})_3]_{\text{aq}}$	1072	24	A1	2	4	2	-	-	-
#4	$[\text{YCl}_4(\text{H}_2\text{O})_2]^-$	1072	26	A1	2	4	2	-	-	-
#5	$[\text{YCl}_5(\text{H}_2\text{O})]^{2-}$	1072	26	A1	2	4	2	-	-	-
#6	$[\text{YF}(\text{OH})(\text{H}_2\text{O})_5]^+$	1072	25	A2	-	-	-	1	-	-
#7	$[\text{YF}_2(\text{H}_2\text{O})_5]^+$	1072	29	A3	-	-	-	1	-	-
#8	$[\text{YF}_3(\text{H}_2\text{O})_4]_{\text{aq}}$	1072	29	A4	-	-	-	1	-	-
#9	$[\text{YClF}(\text{H}_2\text{O})_5]^+$	1072	29	A2	2	4	2	1	-	-
#10	$[\text{YCl}_2\text{F}(\text{H}_2\text{O})_4]_{\text{aq}}$	1072	29	A2	2	4	2	1	-	-
#11	$[\text{YClF}_2(\text{H}_2\text{O})_4]_{\text{aq}}$	1072	27	A3	3	4	1	1	-	-
#12	$[\text{Y}(\text{H}_2\text{O})_7]^{3+}$	1072	29	A1	-	-	-	-	-	-
#13	$[\text{YCl}(\text{H}_2\text{O})_6]^{2+}$	1447	27	B1	3	5	2	-	-	-
#14	$[\text{YCl}_2(\text{H}_2\text{O})_5]^+$	1447	27	B1	3	5	2	-	-	-
#15	$[\text{YCl}_3(\text{H}_2\text{O})_4]_{\text{aq}}$	1447	27	B1	-	-	-	-	-	-
#16	$[\text{YF}(\text{H}_2\text{O})_7]^{2+}$	1447	24	B2	-	-	-	2	4	2
#17	$[\text{YF}_2(\text{H}_2\text{O})_5]^+$	1447	27	B2	-	-	-	2	4	2
#18	$[\text{YF}_3(\text{H}_2\text{O})_4]_{\text{aq}}$	1447	25	B2	-	-	-	2	4	2
#19	$[\text{YClF}(\text{H}_2\text{O})_5]^+$	1447	25	B2	3	5	2	2	4	2
#20	$[\text{YCl}_2\text{F}(\text{H}_2\text{O})_5]_{\text{aq}}$	1447	25	B2	-	-	-	2	4	2
#21	$[\text{YClF}_2(\text{H}_2\text{O})_5]_{\text{aq}}$	1447	27	B2	-	-	-	2	4	2
#22	$[\text{Y}(\text{H}_2\text{O})_8]^{3+}$	1447	27	B1	-	-	-	-	-	-