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Solid Earth Discussions

Interactive comment on "Yttrium speciation in subduction zone fluids from *ab initio* molecular dynamics simulations" *by* Johannes Stefanski and Sandro Jahn

Anonymous Referee #1

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This is an excellent manuscript on predicting the strengths of the complexes of Y with OH, F, and Cl. A great strength of the manuscript is that it takes pains to transform the results of the molecular simulations to thermodynamic equilibrium constants, so that the results can be compared with traditional thermodynamic estimation techniques.

This manuscript should be accepted with just minor corrections, as follows:

line 429....does not yield stable Ho/Y complexes... This statement seems to indicate that the authors think that a logK of less than zero is "not stable". It only shows that the complex is weak...a value of logK=0 has no special significance as it is a standard state quantity. The authors need to be more careful about the use of term "stable".

lines 450-451: again this confusing use of the word "stable". Just because the logK values are different doesn't mean F will predominate over Cl complexes. As the authors show in Fig. 12, the final concentration of a complex in a fluid depends also on the amount of available ligand. And that ligand might be taken up by much more abundant cations than Y3+, e.g. Mg2+ or Ca2+, and so on.

lines 485-490: Also, MgF+ and CaF+ could take up all the F-

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