

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

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We would like to thank the reviewer for useful comments. Here is our point by point reply (line numbers in the answers refer to the revised manuscript).

comment: 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".

C1

answer: We thank the reviewer for making this valid point. We revised this notation in all paragraphs where a misleading interpretation could arise for the reader (see lines 8-10, 273, 293, 361, 382, 434, 456, 474). Stability is now used either in the context of mechanical stability during the MD simulation or of specific thermodynamic conditions.

comment: 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.

answer: See answer to previous comment.

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

answer: We further discuss the competition of different metal cations for F⁻ in line 532.

Interactive comment on Solid Earth Discuss., <https://doi.org/10.5194/se-2019-195>, 2020.

C2