

Supplementary Material

On the aqueous solvation of $\text{AsO}(\text{OH})_3$ vs $\text{As}(\text{OH})_3$. Born-Oppenheimer molecular dynamics density functional theory cluster studies.

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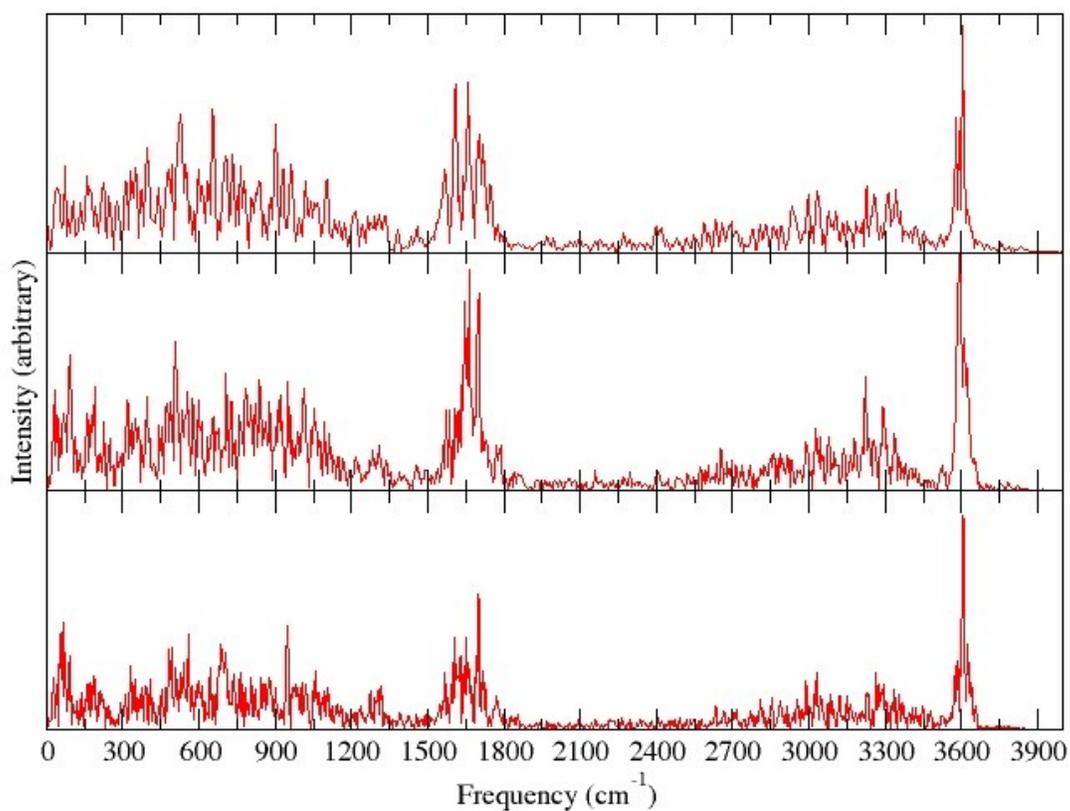


Fig S1. Vibrational spectra of the microhydrated $\text{AsO}(\text{OH})_3$ species calculated using (top) 5 ps, (middle) 7 ps and (bottom) 10 ps of simulation after thermalization has been achieved.

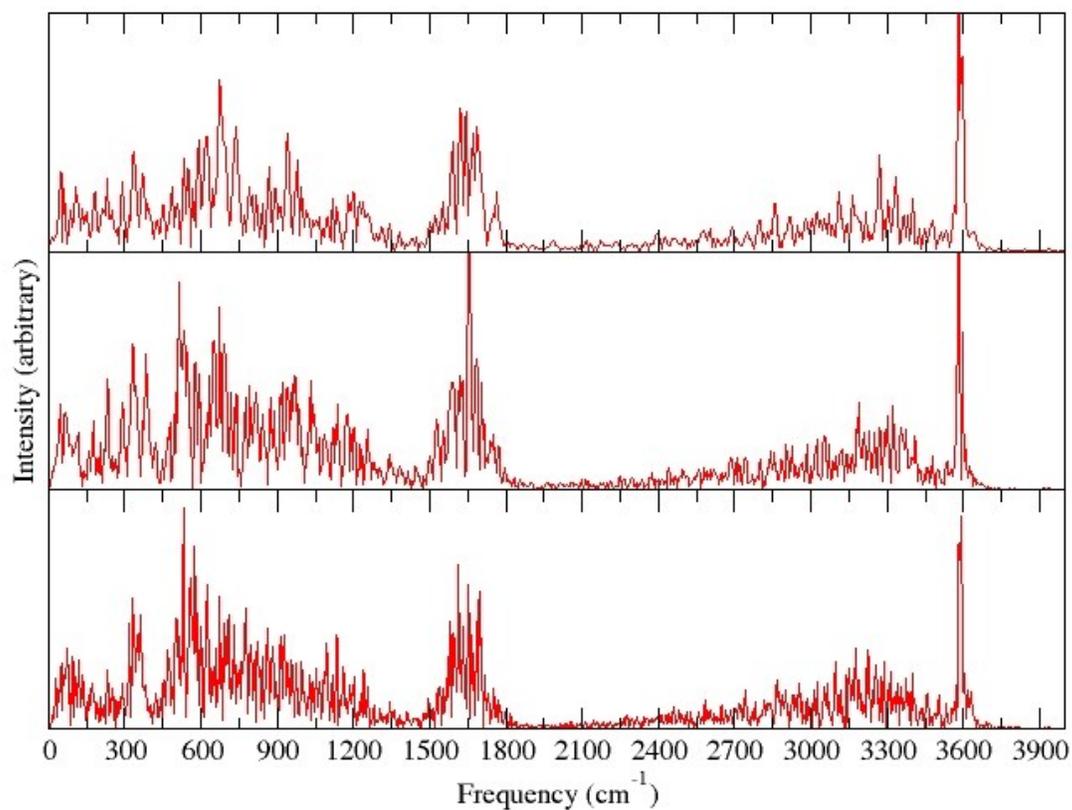


Fig S2. Vibrational spectra of the microhydrated As(OH)_3 species calculated using (top) 5 ps, (middle) 7 ps and (bottom) 10 ps of simulation after thermalization has been achieved.

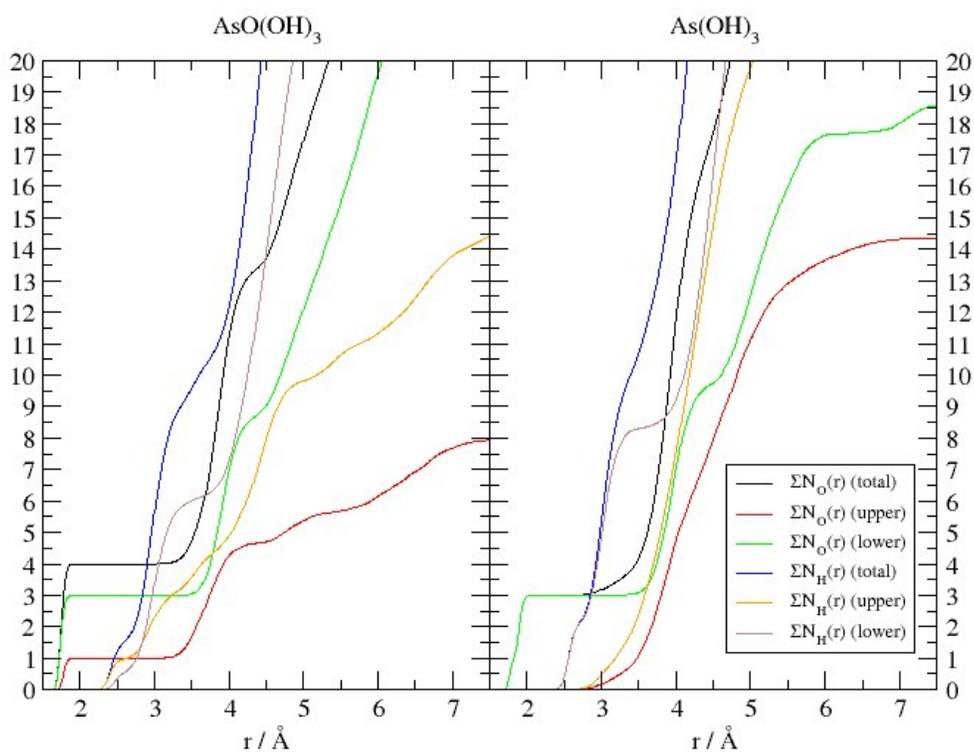
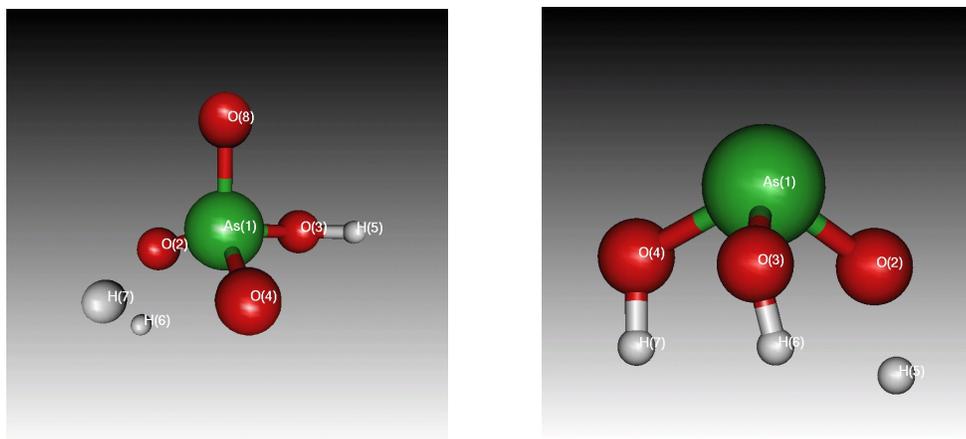


Fig S3. Frames of reference to define the “upper” and “lower” hemispheres for $\text{AsO}(\text{OH})_3$ (top left) and $\text{As}(\text{OH})_3$ (top right), with the plane of O(2), O(3) and O(4) and the origin at As in both cases. The cumulative numbers of oxygens, $\Sigma N_{\text{O}}(r)$, and hydrogens, $\Sigma N_{\text{H}}(r)$, are depicted as functions of the As-O and As-H distances in the graphs at the bottom.

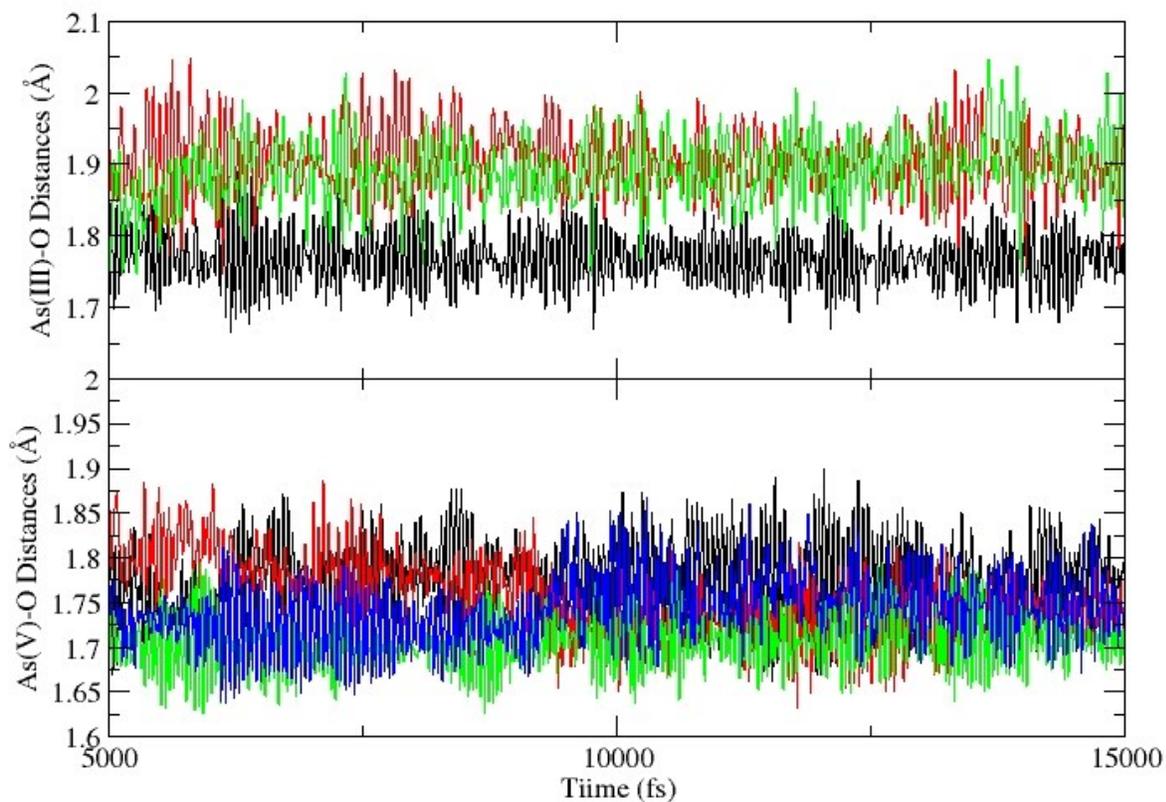


Fig S4. Evolution of the As(III)-O (top) and As(V)-O distances (bottom) for the solute-bound oxygens; only the last 10 ps of the simulations are shown. Note the equivalence of the four oxygen atoms for the As(V) case associated with the HAsO_4^{2-} dominant species.