Supplementary Material

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

A. Ramírez-Solís, J. I. Amaro-Estrada, C. I. León-Pimentel, J. Hernández-Cobos, S. E. Garrido-Hoyos and H. Saint-Martin

![Fig S1](image_url)

Fig S1. Vibrational spectra of the microhydrated AsO(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 AsO(OH)$_3$ (top left) and As(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, $\sum N_o(r)$, and hydrogens, $\sum N_H(r)$, 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.