A theoretical study of $[Be,(H2O)_n]^{2+}$, $[BeOH,(H_2O)_{n-1}]^{+}$ and $[Be(OH)_2,(H_2O)_{n-2}]$ aggregates (n=1–6). Incidence of the first hydration shells on the hydrolysis reactions of Be^{2+} and $BeOH^{+}$ systems

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Ab initio results regarding the incidence of the first and part of the second hydration shell on the hydrolysis reaction of solvated Be^{2+} and $BeOH^{+}$ systems are presented. These results exhibit that the first shells strongly reduce the energy cost of the $Be^{2+} \rightarrow BeOH^{+} + H^{+}$ reaction, however, this reaction remains strongly exothermic. For the $BeOH^{+} \rightarrow Be(OH)_2 + H^{+}$ reaction, the first shells have considerably less incidence on it. This reaction is endothermic and its Helmholtz free energy cost is of the same order of magnitude as that experimentally reported in water.