Influence of nitrogen donor ligands on water exchange at solvated Be^{2+}-Ions $[Be(L)(H_2O)_3]^{2+}$

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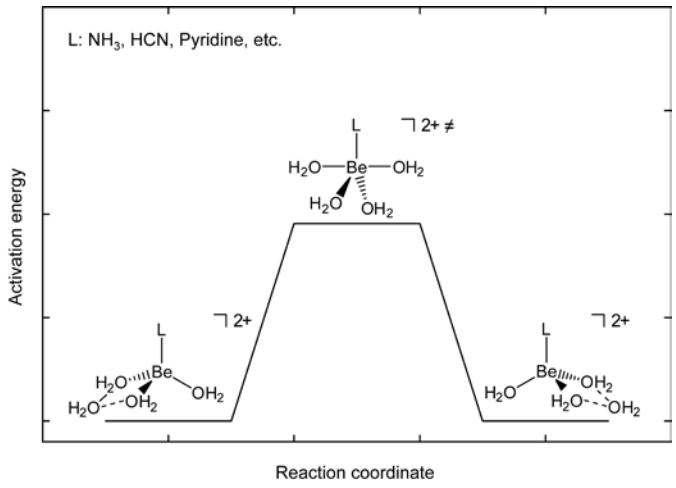
Beryllium has important technological applications, but little is known about its biological and health-related properties and its reactivity. Effects on the human organism are still unknown and up to now there is no chelating agent for beryllium available for medical use.[1]

Solvent exchange reactions on solvated metal ions are one of the simplest processes a metal center can undergo. Even though these reactions don't yield any chemical conversions, they do contribute to our understanding of the reactivity of metal ions in different coordinating environments.[2]



While experimentally feasible, beryllium toxicity prevents extensive studies of ligand exchange reactions. For this reason we applied DFT methods (B3LYP/6-311+G**) to study the water exchange reactions on $[Be(L)(H_2O)_3]^{2+}$ (L: NH_3, HCN, Pyridine etc.), laying emphasis on examining the effects of different hybridizations, proton affinities etc. on the reaction mechanism.

[1] M. D. Rossman, O. P. .Preuss, M. B. Powers, *Beryllium Biomedical and Environmental Aspects*, Williams & Wilkins, Baltimore, **1991**.
[2] R. Puchta, E. Pasgreta, R.van Eldik, *Adv. Inorg. Chem.*, **2009**, *61*, 523 - 571.