Removing Tritium from Nuclear Cooling Water:
Quasi-chemical Theory of Hydroxide and Tritium Oxide

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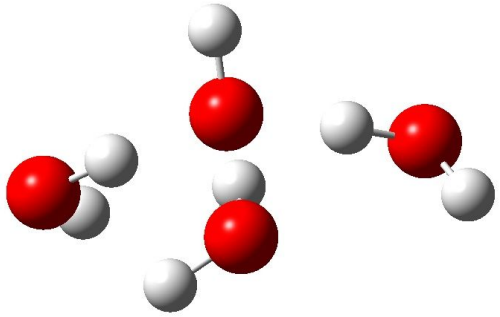
Quasi-chemical theory is utilized to find the solvation free energy of OH^- and OT^-. This theory considers the solvation free energy as a series of contribution from HO $[H_2O]_n^-$ and TO $[H_2O]_n^-$ clusters. B3LYP/6-311G+(2d,p) was used to find the electronic energy. A conjugate gradient method was used to find the optimum energy and geometry. Real frequencies verified that a minimum was found. Vibrational and rotational constants are used to calculate the free energy of the clusters using harmonic and anharmonic approximations. The thermodynamic results will be used to investigate how the structure of a material affects isotope exchange and selectivity. From this study of hydroxide and tritium oxide, it is determined that $HO[H_2O]_3$- and TO $[H_2O]_3$- are the most stable structure of molecules.



HO $[H_2O]_3^-$