

The Thermodynamics and Kinetics of Isotope Exchange

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Tritium, a radioactive isotope of hydrogen, has a half-life of over 12 years. Replacement of a proton with tritium in many biochemical reactions affects reaction rates and the body's chemistry. In mice, ingestion of tritiated water results in death. These health hazards and society's need for energy has sparked interest in developing efficient ways to remove tritium from nuclear cooling water.

Macrobicyclic amines have both internal and external binding sites. Protons can bind to the external binding site and then be transported into the amine. Experimental studies have observed a faster rate for a deuteron entering the amine than a proton. This suggests that these structures could be used to selectively trap tritium.

Our thermodynamic studies have found a preference for the interior binding site in 444 and 666 macrobicyclic amine cages. Exchange of a proton at the outside binding site with tritium from tritiated water is also thermodynamically favorable. With these positive thermodynamic results, we have turned our attention to kinetics. A simple model reaction will be considered as an example of how to find transition state rate constants. We plan to use these transition state methods to find the rate of isotope exchange in these systems.