Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Seminar

Enhanced rate of H-atom transfer to a Mn non-heme complex in water as compared to acetonitrile

Adabala Venkata Snehit

TIFR, Hyderabad

Solvents may profoundly affect enzymatic reactions by modulating reaction rates and selectivity via explicit interactions (e.g. hydrogen bonding if protic) and/or dielectric stabilisation. In biomimetic chemistry, one tries to replicate the enzymatic reaction by mimicking only the active site. In this study, Prof. Sayam Sen Gupta's research group found out that the rate of H-atom transfer from 1-benzyl-1,4-dihydronicotinamide to a Mn(V)-oxo b-TAML complex is enhanced by 20,000-fold on moving from acetonitrile to water. Our extensive calculations suggest that this reaction is an example of 2-state reactivity, where the ground states of the reactant and product have different spin multiplicities. We further found out that the highest energy point along the reaction coordinate is the crossing point between the two spin surfaces, where the proton is still close to the reactant configuration, but an electron has already transferred. This charge-separated crossing point is preferentially stabilised in water as compared to acetonitrile, resulting in the major solvent dependence of the rate of the H-atom transfer.

Wednesday, May 20th 2026

14:00 Hrs (Tea / Coffee 13:45 Hrs)

CR-1, TIFRH