Quantum catalysis in enzymes—beyond the transition state theory

Papers of a Discussion Meeting organized and edited by Leslie Dutton FRS, Nigel Scrutton, Mike Sutcliffe and Andrew Munro

Introduction. Quantum catalysis in enzymes: beyond the transition state theory paradigm
P. L. Dutton, A. W. Munro, N. S. Scrutton & M. J. Sutcliffe

Darwin at the molecular scale: selection and variance in electron tunnelling proteins including cytochrome c oxidase
C. C. Moser, C. C. Page & P. L. Dutton

The role of enzyme dynamics and tunnelling in catalysing hydride transfer: studies of distal mutants of dihydrofolate reductase
L. Wang, N. M. Goodey, S. J. Benkovic & A. Kohen

Protein motions during catalysis by dihydrofolate reductases

Linking protein structure and dynamics to catalysis: the role of hydrogen tunnelling
J. P. Klinman

Quantum catalysis in B12 dependent methylmalonyl-CoA mutase: experimental and computational insights
R. Banerjee, A. Dybala-Defratyka & P. Paneth

Unusual origins of isotope effects in enzyme-catalysed reactions
D. B. Nortrup

Proton-coupled electron transfer: the mechanistic underpinning for radical transport and catalysis in biology
S. Y. Reece, J. M. Hodgkiss, J. A. Stubbe & D. G. Nocera

Hydride transfer catalysed by Escherichia coli and Bacillus subtilis dihydrofolate reductase: coupled motions and distal mutations
S. Hammes-Schiffer & J. B. Watney

Hydrogen tunnelling in enzyme-catalysed H-transfer reactions: flavoprotein and quinoprotein systems
M. J. Sutcliffe, L. Masgrau, A. Roujeinikova, L. O. Johannissen, P. Hothi, J. Basran, K. É. Ranaghan, A. J. Mulholland, D. Leys & N. S. Scrutton

An analysis of reaction pathways for proton tunnelling in methylamine dehydrogenase

Transition state theory can be used in studies of enzyme catalysis: lessons from simulations of tunnelling and dynamical effects in lipoxygenase and other systems
M. H. M. Olsson, J. Mavri & A. Warshel

Protein dynamics and catalysis: the problems of transition state theory and the subtlety of dynamic control
R. W. C. Ingle, B. K. Holeman & S. D. Schwartz

Exploring biomolecular machines: energy landscape control of biological reactions
J. N. Onuchic, C. Kobayashi, M. Miyashita, P. Jennings & K. K. Baldridge

Summarizing lecture: factors influencing enzymatic H-transfers, analysis of nuclear tunnelling isotope effects and thermodynamic versus specific effects
R. A. Marcus