

This volume contains papers based on presentations at the International Conference “2001 an Isotope Odyssey: New Applications for the New Millennium”, which was held June 24–29, 2001 in Zakopane, Poland. The conference was the second in the new European series originated in Carryle-Rouet, France in 1999 and held biennially to alternate with the Gordon Research Conferences “Isotopes in Physical and Life Sciences” that are held during even years in Ventura, CA, U.S.A. The conference gathered about 80 active participants from nearly 20 countries with Polish (24 participants) and American (20 participants) delegations being the most abundant.

It is important to note that this volume, while constituting the formal proceedings of the conference, does not necessarily reflect the true scope of the conference. It is a collection of peer reviewed papers contributed by those presenters who elected to do so. The organizers, while encouraging participants to submit their work for publication in this supplement, did not require submission or exert any other pressure. Thus, for the completeness of the record of the conference program we list here all lectures, which were by invitation of the organizing committee following advice from the session chairs:

1. Theory of tunneling and isotope effects, session chaired by Donald G. Truhlar (University of Minnesota, U.S.A.) “Theory of isotope effects and tunneling”; Zorka Smedarchina (National Research Council of Canada) “Multiple proton tunneling along hydrogen-bond bridges: theory vs. experiment”; Jose L. Luch (Universitat Autònoma De Barcelona, Spain) “Theoretical studies of some isotope effects due to tunneling”;
2. Calculations of isotope effects on enzymic reactions, session chaired by Ian H. Williams (University of Bath, U.K.) “Computational studies of compression effects on enzyme-catalysed methyl transfer”; Jiali Gao (University of Minnesota, U.S.A.) “Combined QM/MM calculation of kinetic isotope effects in enzymatic reactions”; Vincente Molinar (Universitat Jaume I Castello, Spain) “QM/MM kinetic isotope calculations on enzymic reactions”; Paul Berti (McMaster University, Hamilton, Canada) “Enzymatic transition states: the difference between being an oxocarbenium ion and just looking like one”;
3. Tunneling isotope effects – practice, session chaired by Judy P. Klinman (University of California-Berkeley, U.S.A.) “Hydrogen tunneling as a probe of protein dynamics”; Amnon Kohen (University of Iowa, U.S.A.) “Probing enzymatic H-transfer via H/D/T KIEs and their temperature dependency”; Ruma Banerjee (University of Nebraska, U.S.A.) “Quantum mechanical tunneling in H-atom transfer by B12-dependent methylmalonyl-CoA mutase”; Mike Sutcliffe (Leicester University, U.K.) “Theoretical studies of hydrogen tunnelling in enzymes”;
4. Isotope effects on enzymic reactions – practice, session chaired by Vern Schramm (Albert Einstein College of Medicine, U.S.A.) “Binding and equilibrium isotope effects in enzymatic reactions”; Alvan C. Hengge (Utah State University, U.S.A.) “Enzymatic reactions of phosphothioates”; Paul F. Cook (University of Oklahoma,

- U.S.A.) “Stability of the oxalacetate intermediate in the tartrate dehydrogenase-catalyzed D-malic enzyme reaction”; Beniamin Horenstein (University of Florida, U.S.A.) “Mechanistic variation in the glycosyltransfer of N-acetylneuraminic acid”; Daniel Quinn (University of Iowa, U.S.A.) “Computational and experimental studies of transition state. Structure in cholinesterase catalysis”;
5. Global isotope cycles, session chaired by Marion H. O’Leary (California State University, Sacramento, U.S.A.); Hans-Ludwig Schmidt (Technische Universität Munchen, Germany) “Principles and regularities in the formation of the intermolecular and intramolecular isotope distributions in biological systems”; Kazimierz Rożański (AGH, Cracow, Poland) “Isotope effects in the global hydrological cycle”;
  6. Kinetic isotope effects, session chaired by Arnold Jarczewski (A. Mickiewicz University, Poznań, Poland) “Factors influencing kinetic isotope effects in some proton transfer reactions in aprotic solvents”; Joseph J. Gajewski (Indiana University, U.S.A.) “Mechanisms of synthetically useful reactions: carbonyl additions”; Maurice Kreevoy (University of Minnesota, U.S.A.) “The relation between geometric and other isotope effects”; Ken Westaway (Laurentian University, Canada) “Isotope effects to model  $S_N2$  transition states”;
  7. Isotope effects in spectroscopies, session chaired by Poul Eric Hansen (Roskilde University, Denmark) “New isotope effects as observed by NMR”; Hans H. Limbach (Freie Universität Berlin, Germany) “NMR-studies of kinetic and geometric hydrogen isotope effects and tunneling”; Ole Faurskov Nielsen (University of Copenhagen, Denmark) “Fast collective dynamics in molecules of biological interest. A Raman spectroscopic studies by isotopic substitution”;
  8. Radiochemistry, session chaired by Olle Matsson (University of Uppsala, Sweden) “Elucidation of reaction mechanisms using kinetic isotope effects of short-lived radionuclides”; Marianna Kańska (Warsaw University, Poland) “Primary and secondary hydrogen isotope effect in the reaction catalyzed by phenylalanine ammonia lyases”; Bengt Långström (P.E.T. Center, Uppsala, Sweden) “Positron emitting tracers – P.E.T. – for non-invasive measurements of *in vivo* biochemistry. Perspectives in medicine and pharmacology”;
  9. Thermodynamic isotope effects, session chaired by Jerzy Szydłowski (Warsaw University, Poland) “Isotope effects on chemical and phase equilibria – yesterday and today”; Gabor Jancsó (Hungarian Academy of Sciences) “Interpretation of isotope effect on the solubility of gases”; Wojciech Dembiński (IChTJ, Warsaw, Poland) “Isotope effects of lanthanide elements in exchange systems”; Alexander Van Hook (University of Tennessee, U.S.A.) “Isotope effects on vapor phase 2nd virial coefficients”.

In addition two other sessions were held: a poster session with over 30 contributions, and a Young Scientists Forum, chaired by Olivier Breas (J.R.C.-I.R.M.M., E.C.) “Usefulness of absolute measurements in linking  $\delta$ -scale to  $SI^1$ ”, which included 7 presentations by Ph.D. students and recent graduates.

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The next conference in this series is planned to be held in Uppsala, Sweden in 2003. For information on this conference contact Prof. Olle Matsson at [ollem@kemi.uu.se](mailto:ollem@kemi.uu.se)

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