

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

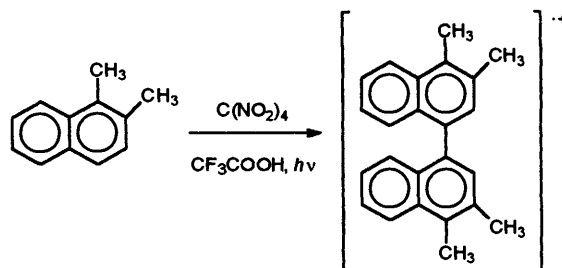
Physical Organic Chemistry

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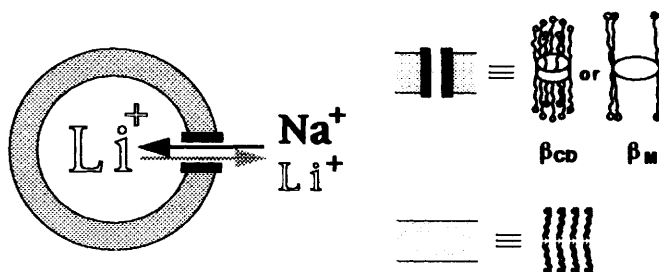
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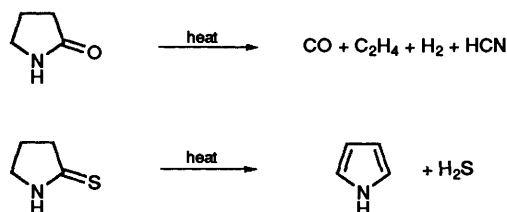
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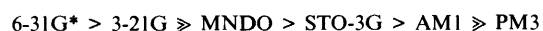
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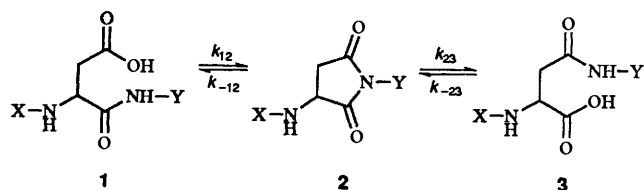
Howard B. Broughton, Stuart M. Green and Henry S. Rzepa

The molecular electrostatic potentials of a series of imidazoles and pyrazoles have been mapped to their respective pK_a values and proton affinities using a backpropagation neural network. Predictions made by the trained network remain sensitive to the quality of the semiempirical and *ab initio* methods used.



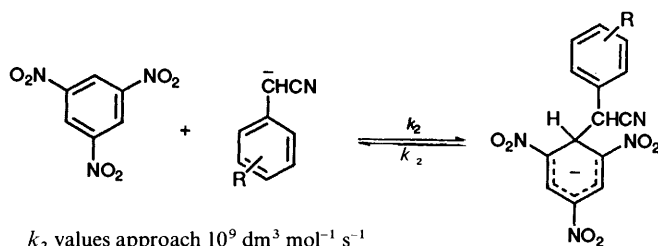
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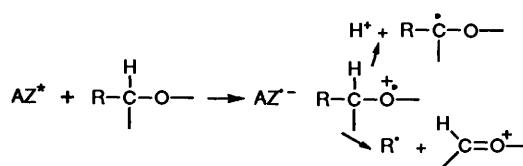
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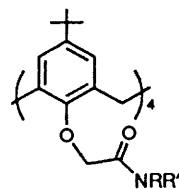
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The radicals are trapped by $AZ^{\cdot -}$ or by acrylonitrile

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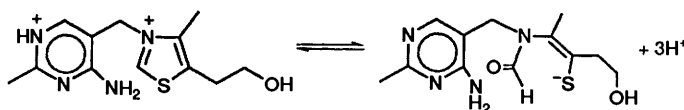
Françoise Arnaud-Neu, Geraldine Barrett, Stefano Fanni, Debbie Marrs, William McGregor, M. Anthony McKervey, Marie-José Schwing-Weill, Victor Vetrogon and Serge Wechsler



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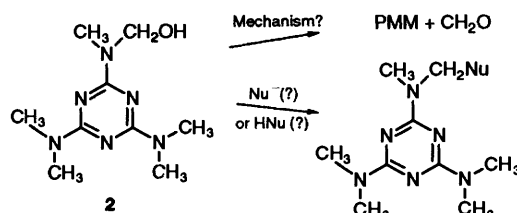
Joachim Herrmann, Wilhelm Knoche and Roland Neugebauer



The mechanism of the hydrolysis of thiamine is studied and equilibria between the ten species involved are determined

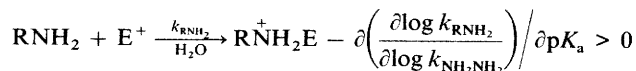
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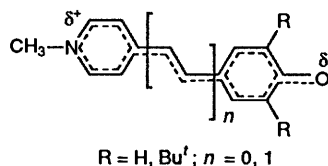
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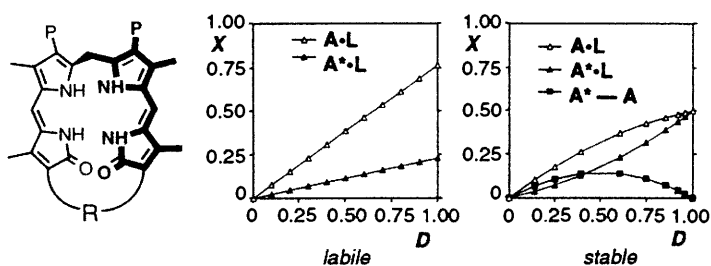
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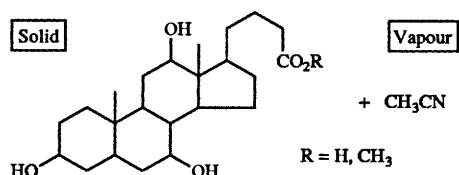
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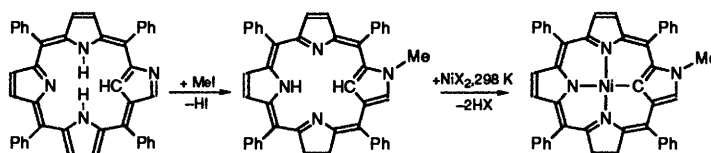
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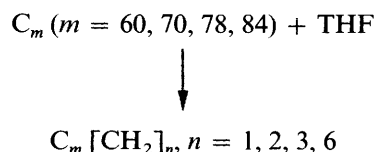
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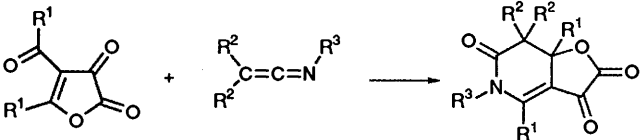
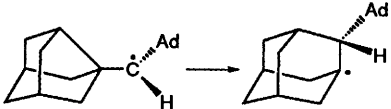
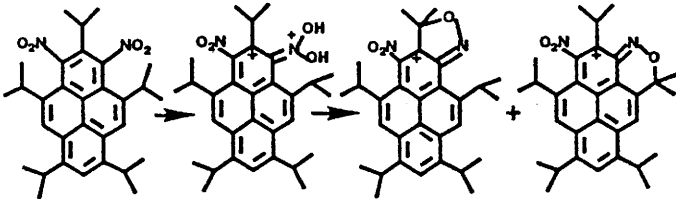
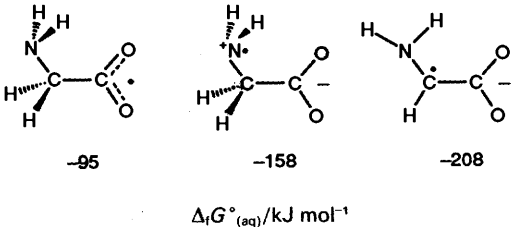


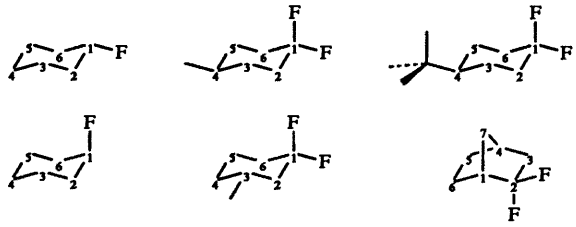
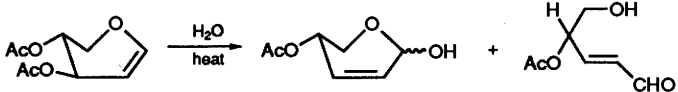
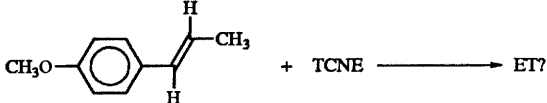
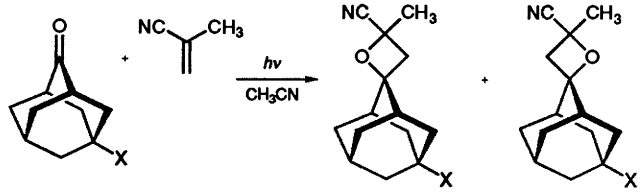
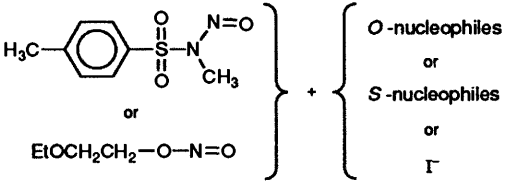
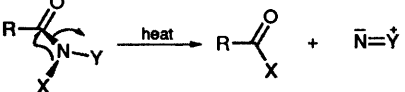
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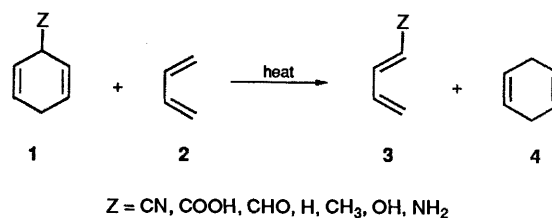
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<p>John S. Lomas</p>	<p>Rearrangement of the 1-adamantyl-3-noradamantylmethyl radical to the 1,2'-biadamantyl radical competes with hydrogen abstraction from solvent</p>
<p>529 Comments concerning solvent effects on chemical processes. Part 7. Quantitative description of the composition dependence of the solvent polarity measure $E_T(30)$ in binary aqueous-organic solvent mixtures</p>	<p>Competitive solvation scheme: $RW_2 + M \rightleftharpoons RWM + W$ $RWM + M \rightleftharpoons RM_2 + W$</p> <p>Observed spectrum in the binary solvent mixture: $\text{spectrum}(X_2) = F_{RWW}(\text{spectrum } RW_2) + F_{RWM}(\text{spectrum } RWM) + F_{RMM}(\text{spectrum } RM_2)$</p>
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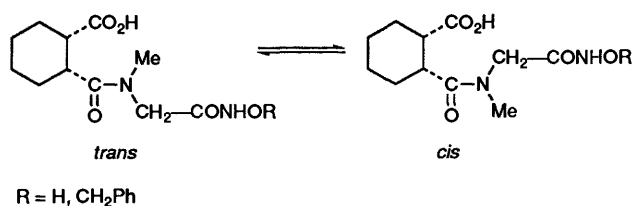
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Miquel Solà, Montserrat Ventura, Cristóbal Segura and Miquel Duran



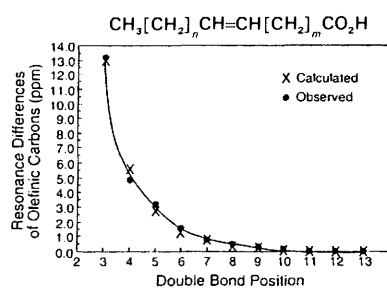
609 Structure and conformation of (1*S*,2*R*)-*cis*-2-[hydroxycarbonylmethyl(*N*-methyl)aminocarbonyl]cyclohexanecarboxylic acid: X-ray, NMR and molecular mechanics studies

Cristina Di Bugno, Spartaco Mauro Colombani, Paolo Dapporto, Raffaello Giorgi and Paola Paoli



615 ¹³C NMR spectroscopy of unsaturated long-chain compounds: an evaluation of the unsaturated carbon signals as rational functions

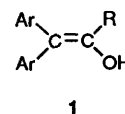
Gerhard Knothe and Marvin O. Bagby



This kind of evaluation also holds for other compounds

621 ¹⁷O and ¹³C NMR spectra of stable simple enols

Joseph Frey, Irina Eventova, Zvi Rappoport, Thomas Müller, Yoshio Takai and Masami Sawada



The ¹⁷O and ¹³C NMR spectra of several simple stable enols **1** were measured in CDCl₃ and in DMSO. Analysis of the SCS and solvent induced shifts is aided by PM3 calculations, and by *ab initio* calculations on the model compound H₂C=CHOH

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NOTE: An asterisk in the heading of each paper indicates the author who is to receive any correspondence.

International Society of Heterocyclic Chemistry



HONG KONG
INTERNATIONAL SYMPOSIUM
ON
HETEROCYCLIC CHEMISTRY

August 13-16 1995

Department of Chemistry, The University of Hong Kong, Hong Kong

Topics

- *Biologically Active Heterocycles
- *Heterocyclic Ligands in Asymmetric Synthesis
- *New Methods of Heterocyclic Synthesis

Plenary Speakers

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D.L. Boger	Scripps Research Institute, La Jolla
C.M. Che	University of Hong Kong
W.H. Pearson	University of Michigan
H. Takaya	Kyoto University
S.M. Weinreb	Pennsylvania State University

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