NMR applied to structure and reactivity in solution

A meeting organised by

NMR Discussion Group *and* Physical Organic Chemistry Group

RSC | Advancing the Chemical Sciences

4 July 2011
GlaxoSmithKline Stevenage, Gunnels Wood Road, Stevenage SG1 2NY,
R&D Lecture Theatre

Introduction

Welcome to this meeting, which aims to present and stimulate discussion on NMR methods for studying structure and reactivity in solution.

We are very grateful to the companies whose logos are on the front page, namely ACD/Labs, Agilent, Bruker, GPE, Jeol, Mestrelab Research and Modgraph, who have enabled this meeting to take place through sponsorship of the meeting. We hope that you will take the opportunity to talk to their representatives who are here today.

We are also grateful to GSK for hosting the meeting, and for making available their excellent facilities.

The meeting has been planned to allow plenty of time for discussion and networking. We hope that you come away from the meeting with fresh ideas and new contacts.

Organising committee:

Mike Williamson, University of Sheffield	NMRDG
Tim Smith, JEOL UK	NMRDG
Craig Butts, Bristol University	POCG
Niek Buurma, Cardiff University	POCG
Ben Bardsley, GSK Stevenage	Local Organiser

Programme

10.30 Registration and coffee

Session 1: Reactions in solution
(Chair: Craig Butts)

11.00 Mathias Nilsson, University of Manchester
New NMR tools for reaction monitoring, mixture analysis and structure elucidation
11.35 Quickfire poster 1 Rob Evans, University of Manchester
Estimating diffusion coefficients for small molecules
11.40 Quickfire poster 2 Ralph Adams, University of Manchester
Resolving natural product epimer spectra by chiral matrix-assisted diffusion-ordered NMR spectroscopy
11.45 Quickfire poster 3 Chris Collett, University of St Andrews
Mechanistic studies of NHC mediated reactions
11.50 Quickfire poster 4 Catharine Jones, University of Bristol
Interproton distances from nuclear Overhauser effect (NOE) data
11.55 Quickfire poster 5 Tim Claridge, University of Oxford
1D HOESY sequences for ^{19}F-^{1}H heteronuclear nOe experiments
12.00 Stefan Berger, University of Leipzig
Attempts to observe a Diels-Alder reaction before it happens

12.35 Lunch
13.15 Poster viewing

Session 2: Structure and association in solution
(Chair: Mike Williamson)

14.35 Jonathan Yates, University of Oxford
Computational approaches to NMR-based conformational analysis
15.10 Chris Hunter, University of Sheffield
Association in solution as probed by chemical shifts

15.45 Tea break

16.15 Award of poster prize (sponsored by Mestrelab)
16.25 Craig Butts, University of Bristol
High accuracy NOEs - a tool for small molecule conformational dynamics
17.00 Finish

Abstracts

New NMR tools for reaction monitoring, mixture analysis and structure elucidation

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Mixture analysis by diffusion NMR is a powerful technique that is steadily gaining ground. The standard way to resolve individual component NMR spectra is by diffusion-ordered spectroscopy (DOSY). The highest resolution in the diffusion dimension can be achieved when the (proton) NMR signals are well separated. However, the whole spectrum of a molecular species generally shows identical diffusion behaviour, and this covariance can be effectively exploited to defeat problems with spectral overlap by multivariate methods such as SCORE [1] and LOCODOSY [2] where whole, or parts of, spectra are fitted simultaneously.

NMR spectroscopy can in principle allow every species involved in a chemical reaction to be monitored simultaneously, providing both real-time quantitation and information on chemical structure. Typically this is done by acquiring ^{1}H spectra at regular intervals and monitoring the integrals of diagnostic peaks, but when signals overlap it is often difficult interpret the data obtained.

One way around this is to acquire successive DOSY datasets during the reaction and apply multilinear (where the data vary independently in more than two dimensions) statistical methods to separate the component spectra [3,4]. Provided that each species has a different diffusion coefficient and a different timecourse, the dataset can be decomposed (without prior knowledge of the spectra, reaction kinetics or diffusion behaviour) using the PARAFAC (PARAllel FACtor Analysis) algorithm to yield the spectrum, concentration time course, and diffusional attenuation for each component of the reaction separately.

Finally, pure shift methods suppress the effects of homonuclear couplings to give spectra without multiplet structure (i.e. only one peak per chemical shift), in 1D and 2D spectra such as DOSY [5] and TOCSY [6], improving resolution by an order of magnitude or more.

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[2] A.A. Colbourne, G.A. Morris, M. Nilsson, Journal of the American Chemical Society 133 (2011) 7640-7643.
[3] M. Khajeh, A. Botana, M.A. Bernstein, M. Nilsson, G.A. Morris, Anal. Chem. 82 (2010) 2102-2108.
[4] M. Nilsson, M. Khajeh, A. Botana, M.A. Bernstein, G.A. Morris, Chem. Commun. (2009) 1252-1254.
[5] J.A. Aguilar, S. Faulkner, M. Nilsson, G.A. Morris, Angew. Chem. Int. Ed. 49 (2010) 3901-3903.
[6] G.A. Morris, J.A. Aguilar, R. Evans, S. Haiber, M. Nilsson, J. Am. Chem. Soc. 132 (2010) 12770-12772.

Estimating Diffusion Coefficients for Small Molecules

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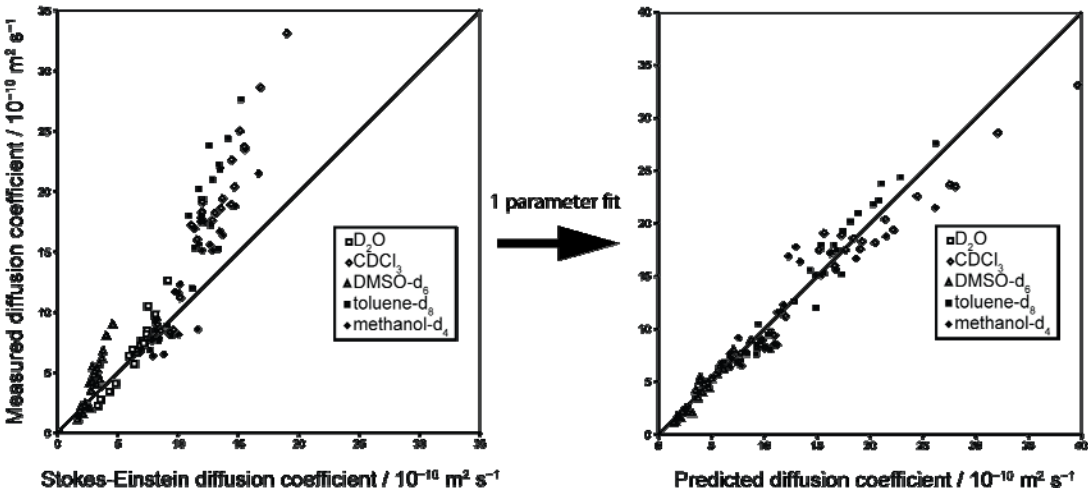
Diffusion-ordered NMR spectroscopy (DOSY)[1] has found increasing use as an analytical tool, capable of identifying the components of mixtures by their individual spectra. However, such techniques have found limited use in quantitative measurement as there is a poor understanding of the relationships between a molecule's size and shape and its diffusion coefficient in solution.

The most basic relationship is that established by the Stokes-Einstein equation[2], which balances the energy of the system to the friction acting on the molecules. However, this relationship becomes less valid as the size of the solute molecules approaches that of the solvent. Various refinements of the original equation have been suggested[3, 4], with that proposed by Chen[5] finding some use in a range of examples[6].

Here a new model is proposed for predicting the diffusion coefficients of small molecules. It has a simple physical basis, is independent of solvent, uses only one adjustable parameter, and is shown to allow diffusion coefficients to be predicted to an accuracy of around 10% using only the solute molecular weight and solvent viscosity.

1. C. S. Johnson, *Prog. Nucl. Magn. Reson. Spectrosc.* **1999**, *34*, 203
2. A. Einstein, *Ann. Phys*, **1905**, *17*, 549
3. J. T. Edward, *J. Chem. Educ*, **1970**, *47*, 261
4. A. Gierer, K. Z. Wirtz, *Naturforsch*, **1953**, *8*, 522
5. H. C. Chen, S. H. Chen, *J. Phys. Chem*, **1984** *88* 5118
6. A. Macchioni *et al*. *Chem. Soc. Rev*, **2008**, *37*, 479



Resolving natural product epimer spectra by chiral matrix-assisted diffusion-ordered NMR spectroscopy

Ralph W. Adams, Juan A. Aguilar, Gareth A. Morris, Mathias Nilsson
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Changes in chemical shift and diffusion coefficient due to the differential inclusion of naringin epimers by β-cyclodextrin allows separation of their signals by high resolution diffusion ordered NMR spectroscopy.

High resolution diffusion-ordered NMR spectroscopy[1] allows the separation of signals from different species based on their diffusion coefficients. In general this requires that the NMR spectra of the components do not have overlapping signals and that the diffusion coefficients are significantly different. Modifying the solvent matrix in which a sample is dissolved can change the diffusion coefficients observed, allowing resolution ("matrix-assisted DOSY").[2] Some matrices can change both diffusion coefficients and chemical shifts. We show here that dissolving the two naturally-occurring epimers of naringin,[3] the component of grapefruit juice responsible for its bitterness, in an aqueous solution of β-cyclodextrin causes both shift and diffusion changes, allowing the signals of epimers to be distinguished. Chiral matrix-assisted DOSY has the potential to allow simple resolution and assignment of the spectra of epimers and enantiomers, without the need for derivatisation or for titration with a shift reagent.

1. C.S. Johnson, *Prog. Nucl. Magn. Reson. Spec.*, 1999, **34**, 203
2. R. Evans, S. Haiber, M. Nilsson and G.A. Morris, *Anal. Chem.*, 2009, **81**, 4548
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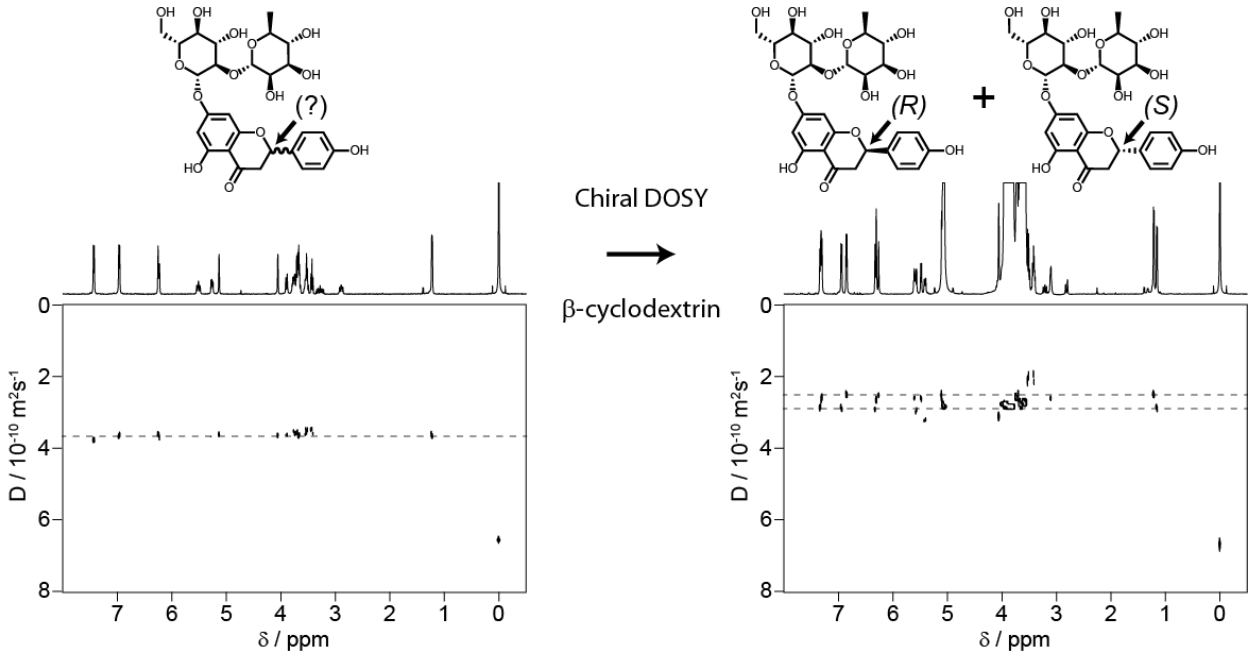

Mechanistic Studies of NHC Mediated Reactions

Chris Collett & Andrew D. Smith
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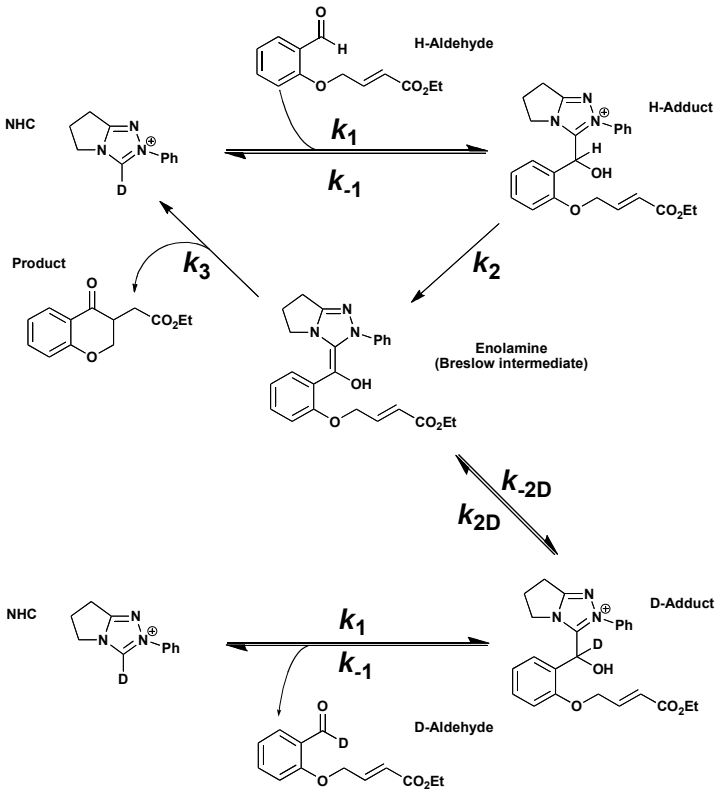
N-heterocyclic carbenes (NHCs) have been shown to act as efficient organocatalysts in a range of synthetically useful transformations. Although a structurally diverse range of NHCs have been synthesised, few studies have been undertaken to relate catalyst structure to their effectiveness both in terms of reactivity and selectivity. The first step of all NHC catalysed reactions involves the *in situ* deprotonation of a triazolium salt to form the carbene. Since this process is dependant on precatalyst pK_a, work was undertaken to determine pK_a values for a range of triazolium salts. These results indicate that factors such as stereodirecting group and secondary ring size have little effect, whilst the *N*-aryl substituent is the most significant influence.

To complement this work studies have been undertaken on the Stetter reaction, involving the formal conjugate addition of an aldehyde into a Michael acceptor, a classic example of an NHC mediated Umpolung transformation. Initially, the adduct formed between the NHC and aldehyde was isolated and fully characterized. Using ^{1}H NMR spectroscopy, it was possible to monitor concentrations of starting materials, intermediates and product over time and construct a reaction profile. From this data, rate constants were determined indicating that the adduct forms quickly, but the subsequent deprotonation to give the enolamine is relatively slow. The enolamine then partitions between the Stetter product and reformation of the adduct. Work is ongoing to prepare a range of these adducts and apply this methodology to chiral NHCs.



Mechanism of the intramolecular Steeter reaction in d_4 methsnol

Interproton Distances from Nuclear Overhauser Effect (NOE) Data

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The determination of accurate interproton distances in solution using NOE data is an area of significant interest and complexity – the large majority of approaches rely on full relaxation matrix analysis of these data. We present a much simpler method that can be used to derive accurate interproton distances from within rigid systems using 1D or 2D NOESY data. Strychnine is used as a model system to test the validity of this method. A comparison between the 1D NOE-derived distances and the best solvent-corrected gas-phase structure of strychnine[1] (Figure 1) produces a mean absolute error of only 2.97% (0.09Å).[2]

A second low-level conformer of strychnine is subsequently identified experimentally by the NOE data and confirmed by computation, thereby demonstrating the potential of accurate NOE measurements to determine minute contributions to structure ensembles in solution.[3]

NOE data is further applied to the small flexible molecule, 4-propylaniline, in the confirmation and prediction of the relative populations of the multiple possible conformers.[4] It is suggested that with the highly accurate interproton distances determined using this method, there is less need for reliance on large numbers of loose restraints, such as scalar couplings, which are typically used in the dynamical analysis of flexible molecules.

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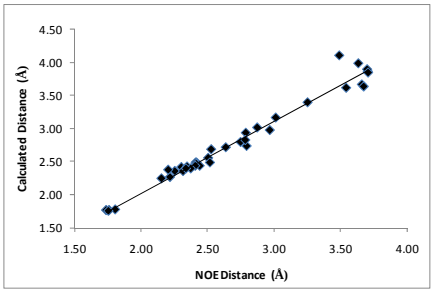
[2] C.P. Butts et al., *Org. Biomol. Chem*., 9 (1), 177-184 (2011).
[3] C.P. Butts, C.R. Jones and J.N. Harvey, *Chem. Comm*., 47 (4), 1193-1195 (2011).
[4] C.R. Jones, C.P. Butts and J.N. Harvey, *Belstein J. Org. Chem.,* 7, 145-150 (2011).



Comparison of calculated distances[1] and NOE-derived distances in strychnine.

1D HOESY sequences for ^{19}F-^{1}H heteronuclear nOe experiments

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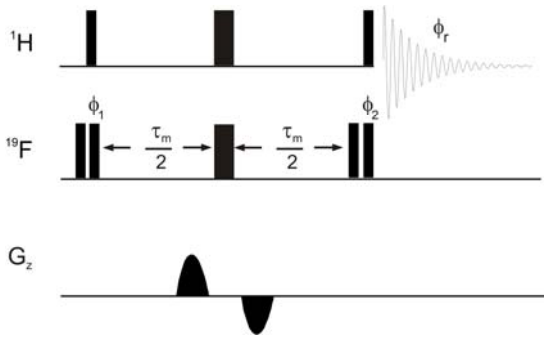
The past decade has witnessed an increasing contribution of fluorine chemistry to the field of pharmaceutical and agrochemical research with up to one quarter of drugs containing at least one fluorine atom. The stereospecific incorporation of fluorine into organic compounds represents an expansive field of research at the interface of bioorganic, chemical biology and medicinal chemistry. As a consequence, methods for the structure elucidation of fluorinated compounds are becoming increasingly important. One approach to this is to employ the nuclear Overhauser effect (nOe) to establish close internuclear relationships between spins and in the context of fluorinated compounds the ^{19}F-^{1}H heteronuclear nOe has considerable potential. Nevertheless, despite recent spectrometer hardware developments, many ^{19}F-^{1}H nOe experiments reported in the literature still utilise the traditional 2D HOESY experiment to observe these interactions , despite this being far from the optimum approach in many cases. Thus, with only a single ^{19}F centre in any compound a ^{19}F detected 2D approach leads to poor ^{1}H resolution in the indirect dimension, with only the single ^{19}F resonance observed directly. For the inverse 2D approach employing ^{1}H observation, the indirect frequency dimension contains only a single fluorine resonance, and there is no need to record a full 2D data set. An optimum approach in such cases is to employ a ^{1}H observe heteronuclear 1D NOE experiment which is time efficient and provides high proton resolution. Herein we describe robust and clean 1D ^{19}F-^{1}H HOESY experiments suitable for qualitative analysis and for quantitative internuclear distance estimates.



Attempts to Observe a Diels-Alder Reaction Before it Happens

Andreas Ossmann, Stefan Berger

Analytical Chemistry, University Leipzig, Germany

We report about an idea to observe chemical reactions at the time where no new chemical bonds are yet formed.

Should one be able to observe the formation of a reaction complex by NMR of the individual reactants? If two reactants A and B form a reaction complex AB, but diffuse apart without having reacted, this event should possibly be detectable by NMR using intermolecular T_1 measurements, Double Quantum spectroscopy (CRAZED) or intermolecular NOE using DPFGSE methods.

In order to proof this concept we have chosen the Diels-Alder reaction which can be easily adjusted in the NMR tube with respect to reaction kinetics. Parameters such as concentration, solvents, temperature, the reactivity of the components and catalysts have been modified. In addition to intermolecular attempts, the intramolecular variant of the Diels-Alder reaction has been tested with special emphasis on the stereochemistry.

The influence of intermolecular interactions on NMR parameters: computational approaches.

Jonathan R. Yates

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In the past few years it has become possible to predict the key NMR parameters (magnetic shielding, EFG, spin-spin coupling) within the planewave-pseudopotential formalism of density functional theory [1]. This allows calculations to be performed for both condensed phases and isolated molecules.

Using a combined experimental and computational approach we have studied the influence of intermolecular interactions on NMR parameters. Such factors include crystal packing, ring currents, hydrogen bonding (both conventional and 'weak') as well as the transmission of *J*-coupling across both hydrogen bonds and 'non-bonding' interactions.

Outstanding challenges involve the role of temperature / dynamics and the influence of weak (dispersion) interactions.

[1] http://www.gipaw.net

Probing solvation thermodynamics using NMR spectroscopy

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Intermolecular interactions in solution are affected by many different factors that have hampered the development of an understanding of molecular recognition at a quantitative level. Our research has focussed on the development of an integrated quantitative appreciation of the relative magnitudes of the various different effects that might influence the intermolecular interactions of a given system. In solution, non-covalent interactions are the result of the competition between solute-solute, solute-solvent and solvent-solvent interactions, and any one of these may dominate in a particular case. Thus an investigation of solvent effects on intermolecular interactions will not only help to delineate this relationship, it can also provide direct insight into the very nature of the forces that govern the behaviour of the liquid state. This presentation will describe some simple NMR experiments designed to quantify the thermodynamic contributions of desolvation to intermolecular complexation in solution.

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High Accuracy NOEs - a Tool for Small Molecule Conformational Dynamics

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'Fact' 1 - NOE data is a powerful tool for qualitative analysis of conformation and stereochemistry.

'Fact' 2 - Quantitative applications of NOEs *e.g.* establishing internuclear distances is risky.

'Fact' 3 - Differentiating structures which contain very similar internuclear distances (say ~10% from each other) or which are influenced by molecular motion which is fast on the NMR timescale (*e.g.* alkyl group rotations) is quite simply foolhardy.

The 'Bristol Hypothesis' - The above facts do not apply to small molecules if you look hard enough.

We have demonstrated that high levels of structural accuracy can be extracted from NOE data for both rigid and conformationally flexible structures.[1] This accuracy has fairly remarkable consequences on the quality of information which can be extracted about both structure and dynamics. We also demonstrate the danger of (i) underdetermining distances *e.g..* the pseudo-atom "correction" (ii) comparing 'accurate' experimental data with calculated energies and the limits of the approach ("the Taxol conundrum"). When you add this to more (and less!) traditional coupling constant measurement and analysis, there is a fascinating story to be told…

[1] C.P. Butts et al., *Org. Biomol. Chem*., 9 (1), 177-184 (2011);
C.P. Butts, C.R. Jones and J.N. Harvey, *Chem. Comm*., 47 (4), 1193-1195 (2011);
C.R. Jones, C.P. Butts and J.N. Harvey, *Belstein J. Org. Chem.,* 7, 145-150 (2011).

Poster abstracts

Spectator Ferrocenyl substituent: pK_a Measurements of 4-Substituted-Pyridinium Ion Derivatives

Casey M. Lam and AnnMarie C. O'Donoghue
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Leading the development of new asymmetric organocatalysts, Fu and co-workers developed a number of organocatalysts derived from 'Planar-Chiral' 4-(dimethylamino)pyridine which have proved to be highly efficient, high yielding and most importantly highly enantioselective for a range of reactions.[1]

As part of a mechanistic investigation of the role of these organocatalysts in several transformations, pK_a values for **1**H$^+$ in DMSO and MeCN employing a 'bracketing buffer' method[2] using appropriate buffer systems have been measured. pK_a values from 12.87 to 19.74 were recorded in MeCN and 3.33 to 9.97 in DMSO. The compounds also tested negative for ion pairing. More importantly no significant substitutent effect of the adjacent ferrocenyl group was observed for all compounds when compared to the 4-substituted pyridine analogues without the ferrocenyl group.

[1] Fu, G. C. *Acc. Chem. Res.* **2004**, *37*, 542.
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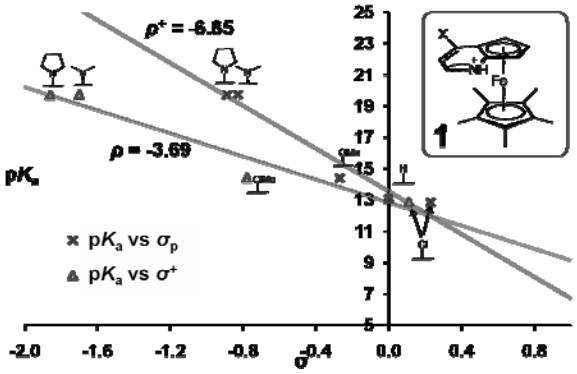

MECHANISM OF NUCLEOPHILIC ORGANOCATALYSIS BY N-HETEROCYCLIC CARBENES: THE BENZOIN CONDENSATION

Richard S. Massey and AnnMarie C. O'Donoghue
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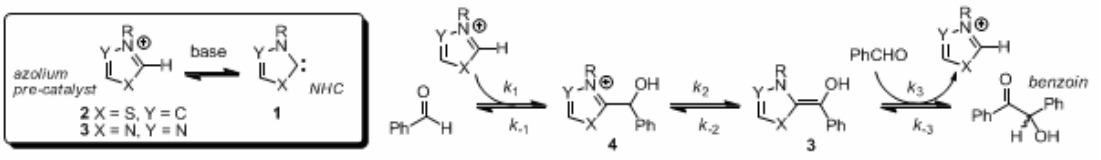
N-heterocyclic carbenes (NHCs (**1**)) are becoming increasingly popular organocatalysts for many transformations, including the benzoin condensation and Stetter reaction. Despite the widespread application of NHCs as organocatalysts, a comparative kinetic study of the catalysis by different NHC families of a given reaction has yet to be made.

We have begun to compare the kinetics of the benzoin condensation, catalysed by thiazolium (**2**) and triazolium (**3**) pre-catalysts. The build-up and decay of reaction species at stoichiometric initial concentrations of pre-catalyst and aldehyde have been followed by ^{1}H NMR spectroscopy in triethylamine buffered d^4-methanol. Hydroxybenzyl adducts (**4**) are observed to accumulate under our reaction conditions and deuterium exchange of the benzylic hydrogen of these species provides indirect evidence for the formation of enamine intermediate (**5**)**.** In the case of the triazolium catalysed reaction, several hydroxybenzyl adducts have been independently isolated and characterised by X-ray crystallography and HSQC NMR spectroscopy. We are currently studying the kinetics of decomposition of these adducts (k_{-1} versus k_2) under our reaction conditions by ^{1}H NMR spectroscopy.



Mechanistic investigations of uncatalysed and osmium(VIII) catalysed oxidation of chlorpheniramine an antihistamine drug by diperiodatoargentate(III) periodate complex in aqueous alkaline medium: a comparative kinetic approach.

Anita Savanur,[1] Shekappa Lamani[2], Shivamurti Chimatadar*
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[2]Department of Chemistry, Karnatak University, PavateNagar Dharwad-58003, India.

The oxidation of chlorpheniramine (CPM), an antihistamine agent, by diperiodatoargentate(III) (DPA) has been investigated spectrophotometrically both in the absence and presence of osmium(VIII) catalyst in alkaline medium at a constant ionic strength of 0.10 mol dm^{-3}. The oxidation products were identified as (4-chloro-phenyl)-pyridin-2yl-methanol, dimethyl amino acetaldehyde and Ag(I). The stoichiometry was same in both the cases, i.e., [CPM]:[DPA] = 1:2. In both the uncatalysed and catalysed reactions, the order with respect to DPA concentration was unity while the order with respect to CPM concentration was < 1 over the concentration range studied. The rate increased with an increase in OH^- ion concentration and decreased with an increase in IO_4^- ion concentration. As the concentration of the catalyst, osmium (VIII), increased the rate of reaction also increased. The order with respect to Os(VIII) concentration was found to be unity. The mechanisms proposed and derived rate laws are consistent with the observed kinetics. Kinetic experiments suggest that $Ag(H_2IO_6)(H_2O)_2$ is the reactive species of oxidant and $[OsO_4(OH)_2]^{2-}$ is the reactive species of catalyst. The activation parameters were evaluated with respect to the slow step of the mechanism.

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Delegates

Ralph Adams
Manchester University

Ian Ashworth
AstraZeneca

Ben Bardsley
GSK Stevenage

Stefan Berger
University of Leipzig

Mike Bernstein
Mestrelab

Andrew Blackaby
Syngenta

Paul Bowyer
Agilent

Craig Butts
Bristol University

Niek Buurma
Cardiff University

Chun-wa Chung
GSK Stevenage

Tim Claridge
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Chris Collett
St Andrews University

Iain Day
Sussex University

Andrew Dolan
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Santi Dominguez
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Georgina Fraser
Imperial College

Ute Gerhard
GSK Stevenage

Andrew Gibbs
Bruker

Chris Hunter
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Jeremy Lea
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