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RESEARCH FRONT: Complexity in Chemistry

Reviews

Emergence and Self-Organization in Chemistry and Biology

David Newth, John Finnigan

Aust. J. Chem. **2006**, *59*, 841–848.

In his seminal 1972 paper *More is Different*, Philip Anderson employed the correspondence between the symmetries of space-time and the conservation laws of physics to state an elegant concept of emergence. In this account we explore some of the notions put forward by Anderson. We show, through the use of examples, how macroscopic symmetry breaking is an important factor in the formation of system-level order from chemical reactions through to the organization of ecosystems.

Classification of Self-Organization and Emergence in Chemical and Biological Systems

Julianne D. Halley, David A. Winkler

Aust. J. Chem. **2006**, *59*, 849–853.

Complex systems science provides a novel way of thinking about dynamic systems through emergence and self-organization approaches. These still poorly comprehended concepts are presented herein with reference to chemical and biological systems.

Current Chemistry

Analyzing Biochemical Pathways Using Neural Networks and Genetic Algorithms

Johann Gasteiger, Martin Reitz, Yongquan Han, Oliver Sacher

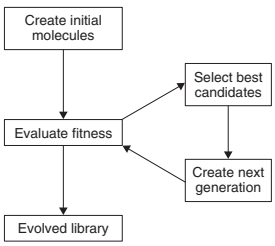
Aust. J. Chem. **2006**, *59*, 854–858.

The well known *Biochemical Pathways* wall chart has been converted into a molecule and reaction database, *BioPath*. A major feature of *BioPath* is that for each transformation the reaction centre and the atoms and bonds directly involved in the bond rearrangement process are marked. This rich database can in turn be mined to find inhibitors for biochemical reactions and to lead to a novel classification of enzymes. A web-based structure and reaction retrieval system, described within, provides a wide range of search methods.

Simulation and Modelling of Chemical and Biological Complex Systems

Mitchell J. Polley, Frank R. Burden, David A. Winkler

Aust. J. Chem. **2006**, *59*, 859–864.



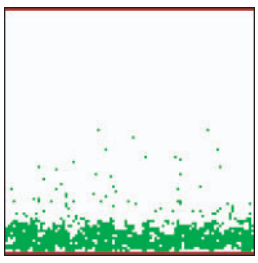
The tools of complex systems science provide alternative methods for modelling chemical and biological systems. Evolutionary methods and agent-based modelling are described and illustrated by examples.

Communications

Cellular Automata Simulations of Vapor–Liquid Equilibria

Paul G. Seybold, Matthew J. O'Malley, Lemont B. Keir, Chao-Kun Cheng

Aust. J. Chem. **2006**, *59*, 865–868.



Employing just two rules, of attraction and gravitation, a stochastic cellular automata model simulates a liquid/vapor interface. Thus, two movement rules represent a minimum to mimic the emergent phase change behaviour.

An Approach Toward Emulating Molecular Interaction with a Graph

Hideaki Suzuki

Aust. J. Chem. **2006**, *59*, 869–873.

In order to mathematically represent molecular/atomic interactions in the chemistries, a topological network is a desirable tool on account of its flexibility. The paper presents a rewiring rule that makes the network conform to the spatial constraints and shows its validity compared to the hard spheres' random walk simulation results. A network governed by the developed rule provides a powerful spatial representation on which we can implement chemical computational machines in silico or abstractly emulate self-organizing phenomena of bio-chemical systems.

Conformational Boosting

Dimitris K. Agrafiotis, Alan Gibbs, Fangqiang Zhu, Sergei Izrailev, Eric Martin

Aust. J. Chem. **2006**, *59*, 874–878.

Comparison of a number of popular conformational sampling techniques for a sample of 59 bioactive ligands shows that a boosting strategy benefits distance geometry methods. Boosting generates a series of conformations which are at least as extended (or compact) as those of the previous iteration and widens the range of geometries sampled in conformational space. The later conformations after boosting have lower RMS deviations from bioactive conformers found in the Protein Data Bank.

Is There a Single 'Best Pool' of Commercial Reagents To Use in Combinatorial Library Design To Conform to a Desired Product–Property Profile?

Jean-François Truchon, Christopher I. Bayly

Aust. J. Chem. **2006**, *59*, 879–882.

Combinatorial libraries are often designed using commercial reagent lists, which are frequently very large. Rather than pruning the reagent lists based on reagent properties, which leads to a single 'best pool' of reagents from which to draw, it is preferable to prune based on the properties of the final products including all the other reagents and the scaffold. Doing this very quickly and efficiently with *GLARE* allows for the comparison of the same starting reagent lists across diverse libraries, showing that the 'best pool' of reagents to draw from differs widely across libraries.

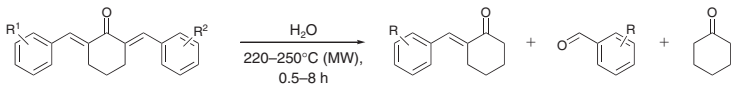
Communication

Reactions of 2,6-Dibenzylidene-cyclohexanone and its Derivatives in High-Temperature Water

Xian-Jun Bi, Luke T. Higham, Janet L. Scott, Christopher R. Strauss

Aust. J. Chem. **2006**, *59*, 883–886.

Derivatives of the title compound were heated in water at 220–250°C under microwave conditions, without added catalyst. Retro-Claisen–Schmidt processes liberated aryl aldehydes. These preliminary experiments highlight multiple roles of high-temperature water as solvent/medium, reactant, and catalyst.



Full Papers

The Synthesis of Membrane Permeant Derivatives of *myo*-Inositol 1,4,5-Trisphosphate

Stuart J. Conway, Jan W. Thuring, Sylvain Andreu, Brynn T. Kvinlaug, H. Llewelyn Roderick, Martin D. Bootman, Andrew B. Holmes

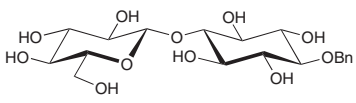
Aust. J. Chem. **2006**, *59*, 887–893.

D-*myo*-Inositol 1,4,5-trisphosphate ($InsP_3$) is an important signalling molecule that is involved in a wide range of cellular processes, such as gene transcription, muscle contraction and cell proliferation. The direct application of $InsP_3$ to the cell to activate its intracellular receptors is not possible, as this polar compound will not passively diffuse across the cell membrane. The syntheses of membrane permeant forms of the natural D-$InsP_3$ and the unnatural L-$InsP_3$ are reported; it is demonstrated that D-$InsP_3$ leads to intracellular Ca^{2+} release following extracellular application, whereas L-$InsP_3$ does not cause Ca^{2+} release.

Glycosynthase-Assisted Synthesis of Some Glycosylated *scyllo*-Inositols

Adrian Scaffidi, Robert V. Stick

Aust. J. Chem. **2006**, *59*, 894–898.



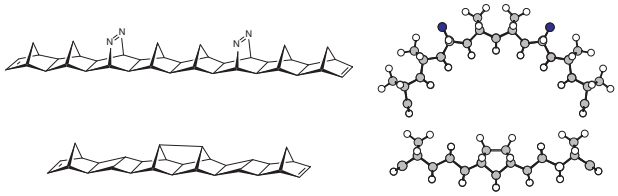
Glycosynthases, mutant glycoside hydrolases, offer a way to synthesize the glycosidic linkage without the problems associated with hydrolases operating in the *trans*-glycosylation mode. The method is applied to three functionalized inositols, two ethers, and one ester, as acceptors, resulting in galactosylated and glucosylated inositols. These results may be useful in elaboration of glucosyl phosphatidyl inositol (GPI) related structures.

Use of a 9,10-Dihydrofulvalene Pincer Cycloadduct as a Cornerstone for Molecular Architecture

Mirta Golić, Martin R. Johnston, Davor Margetić, Austin C. Schultz, Ronald N. Warrener

Aust. J. Chem. **2006**, *59*, 899–914.

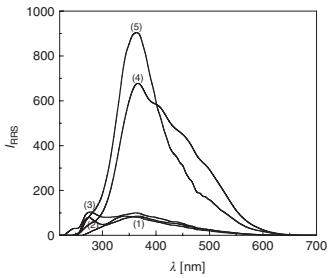
Molecular architectures constructed from polynorbornanes traditionally have curved topology. In this paper, the inclusion of Hedaya's diene into these structures using a building block approach produces linear geometries. The combination of linear and curved molecular sections and effector groups allows useful architectures to be constructed in a straightforward manner.



Resonance Rayleigh Scattering for the Determination of Chlorpromazine and Promethazine

Lanxiang An, Shaopu Liu, Zhongfang Liu, Ling Kong, Xiaoli Hu

Aust. J. Chem. **2006**, *59*, 915–920.



Currently, the quantitative determination of chlorpromazine (CPZ) and promethazine (PZ), both commercially used drugs, involves titration. Here the binding of potassium ferrioxalate to CPZ and PZ is demonstrated to show an enhanced resonance Rayleigh scattering and the method is used to detect levels as low as 6.6 and 10.6 ng mL^{-1} for CPZ and PZ, respectively. Successful application to biological samples is also demonstrated.

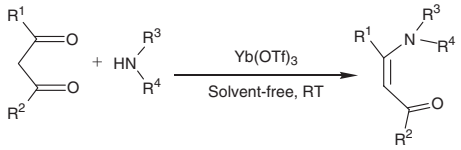
Communications

Efficient Synthetic Method for β-Enamino Esters Catalyzed by $Yb(OTf)_3$ under Solvent-Free Conditions

Ravi Varala, Sreelatha Nuvula, Srinivas R. Adapa

Aust. J. Chem. **2006**, *59*, 921–924.

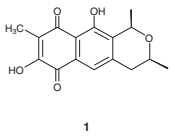
Pharmacologically relevant β-enamino esters have been synthesized by reacting 1,3-dicarbonyl compounds with amines with catalytic amounts of $Yb(OTf)_3$. Reactions proceed smoothly at ambient temperature under solvent-free conditions, with advantages of a small quantity of catalyst, and experimental simplicity. The catalyst can be recovered and reused for applicability in large scale synthesis.



Absolute Configurations of Naturally Occurring Quinones: Ventilagone and Dunnione

Raymond G. Cooke, Emilio L. Ghisalberti, Brian L. Johnson, Colin L. Raston, Brian W. Skelton, Allan H. White

Aust. J. Chem. **2006**, *59*, 925–930.



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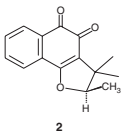

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The outstanding problems regarding the absolute stereochemistry of the naturally occurring naphthoquinones ventilagone **1** and dunnione **2** have been resolved. This result was achieved using modern crystallographic technology on samples first studied in 1980. On the basis of the results reported here, the recent assignment of the absolute stereochemistry of a group of dunnione derivatives requires correction.