

# AUSTRALIAN JOURNAL OF CHEMISTRY

ulated within a te matrix modifies

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The cover represents a photochromic dye encapsulated within a polymer matrix. Steric limitations enforced by the matrix modifies the speed at which the dye can switch between coloured and colourless forms. Learn more in the Current Chemistry article by Evans and Such (p. 825).

#### Foreword

#### Chemistry in Pasteur's Quadrant

Gregory W. Simpson, Thomas H. Spurling

Aust. J. Chem. 2005, 58, 823-824.



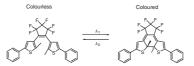
Chemistry has been a strength of the Australian government research organization CSIRO since the 1920s. Contemporaneous with the advent of a new division, Molecular and Health Technologies, this issue of the *Australian Journal of Chemistry* focusses on current CSIRO chemical research.

#### **Current Chemistry**

#### Research Trends in Photochromism: Control of Photochromism in Rigid Polymer Matrices and other Advances

Richard A. Evans, Georgina K. Such

Aust. J. Chem. 2005, 58, 825-830.



Recent advances in the use of thermally irreversible (P type, example shown) and thermally reversible (T type) photochromic dyes are reviewed. Their uses as molecular switches and a new method of controlling colouration switching speed by manipulating the viscosity, or glass transition temperature of the surrounding polymer matrix, are discussed.

#### **Rapid Communications**

#### Temperature-Dependent Cooperative Coiling of Helical Conformers of Enantiopure Oligo(Tertiary Phosphines)

Gerhard F. Swiegers, S. Bruce Wild

Aust. J. Chem. 2005, 58, 831-833.

Many naturally occurring and synthetic molecules adopt a helical form in solution. Most high molecular mass polymers do not. What then is the critical chain length for a given helix inversion barrier that separates this conformation divide?

# Construction of the 1,2,3,4-Tetrahydro-1,4,6,2-oxathiazaphosphorine Ring System

Wynona M. Johnson, Kathleen A. Turner

Aust. J. Chem. 2005, 58, 834-836.

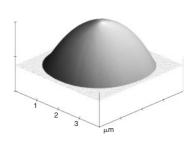
In seeking to provide scaffolds and building blocks for the development of new pharmaceuticals and agrochemicals, the title ring systems were prepared. The reaction of the sodium salt of diethyl mercaptomethylphosphonate with nitrile oxides, followed by cyclization of the resulting hydroximinoyl sulfide, yields the oxathiazaphosphorines. The stability of these systems is also investigated.

#### **Full Papers**

#### Interaction Forces Between Colloidal Silica in Aqueous Inorganic and Natural Organic Electrolyte Solutions

Robert F. Considine, Calum J. Drummond, David R. Dixon

Aust. J. Chem. 2005, 58, 837-844.



To further understand their interactions, hence optimize their roles in a variety of industrial and environmental processes, atomic force microscopy is used to measure the force of interaction between pairs of silica colloids in aqueous inorganic and natural organic electrolyte solutions. The results are interpreted in terms of DLVO theory, specific surface adsorption, and the intermolecular interactions of natural organic matter.

#### Evaluation of Aqueous Extracts from Elast-Eon Polymers for Methylene Dianiline (MDA) by High-Performance Liquid Chromatography (HPLC)

Ramasri Mudumba, Ajay D. Padsalgikar, Stuart W. Littler

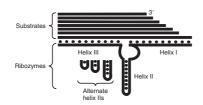
Aust. J. Chem. 2005, 58, 845-850.

Degradation resistance is a critical performance parameter for medical implants. Polyurethane is a common implant material but in vivo polyurethanes are susceptible to enzymatic degradation and release of MDA. The title polymer, a high silicone content polyurethane that notably does not require additives during synthesis, is shown here to also possess remarkable stability against oxidation and sterilization processes.

#### Influence of Helix Length on Cleavage Efficiency of Hammerhead Ribozymes

Philip Hendry, Maxine J. McCall, Trevor J. Lockett

Aust. J. Chem. 2005, 58, 851-858.

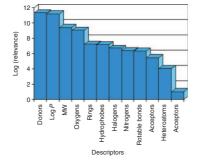


Some RNA molecules fold intramolecularly and cut at specific sites, allowing the molecule to be engineered for binding and cleaving a separate RNA molecule at a desired position. This study reports the in vitro cleavage kinetics of a number of RNA substrates by a range of *trans*-acting hammerhead ribozyme derivatives. The kinetics are controlled by interactions between double helices I and II, with cleavage rates modified by the lengths of both helices and the number of unpaired nucleotides overhanging helix I in either ribozyme or substrate strands.

#### Predictive Human Intestinal Absorption QSAR Models Using Bayesian Regularized Neural Networks

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

Aust. J. Chem. 2005, 58, 859-863.



With the view to improving the efficiency of the drug development process, a predictive model of intestinal absorption data is reported that uses several types of molecular descriptors and a non-linear Bayesian regularized neural network. The model allowed mapping of the most relevant descriptors.

## Synthesis of Some 4-Oxothiochromenes and Related Compounds

Andris J. Liepa, Oanh Nguyen, Simon Saubern

Aust. J. Chem. 2005, 58, 864-869.

A new synthesis pathway for thiochromones with an amino substituent in the 2-position, as an alternative to the route of reacting a 2-bromothiochroman with an amine, is described. A simple one-step synthesis employs both electrophilic and nucleophilic reactivity.

Preparation of 1-[(3-Trifluoromethyl)-phenyl]-3,4-dihydro-2(1*H*)-pyridinone Derivatives from Aza Annulation Reactions of *N*-[(3-Trifluoromethyl)-phenyl]-Substituted Enaminones

The synthesis of some potential phytoene desaturase-inhibiting herbicides that incorporate the title pyridinone-derived structural motif (general structure A) is investigated. The synthesis makes particular use of cyclization reactions of enaminone derivatives with acryloyl chloride, and other alkene- and alkyne-derived electrophiles.

Abdelselam A. Ali, Kevin N. Winzenberg

Aust. J. Chem. 2005, 58, 870-876.

#### Nitrile Oxide Cycloaddition Chemistry Using Benzotriazole as a Steric Auxiliary

G. Paul Savage, Gregory T. Wernert

Aust. J. Chem. 2005, 58, 877-881.

The 1,3-dipolar cycloaddition reaction of nitrile oxides with carbon dipolarophiles yields  $\Delta^2$ -isoxazolines and isoxazoles, themselves useful precursors to a whole range of 1,3-disubstituted compounds. However, nitrile oxides often dimerize to furoxans and hamper this process. Here, bis(benzotriazol-1-yl)acetonitrile oxide (left) is synthesized and found to undergo cycloaddition reactions without dimerization.

### Synthesis of N-Substituted $\gamma$ -Methylene $\gamma$ -Lactams

Raju Adhikari, Dionne A. Jones, Andris J. Liepa, Roland H. Nearn

Aust. J. Chem. 2005, 58, 882-890.

N-substituted cyanoacetamides were condensed with 1,2-diketones under base catalysis to form  $\gamma$ -hydroxy  $\gamma$ -lactams. Treatment of these lactams with acids gave novel fungicidal  $\gamma$ -methylene  $\gamma$ -lactams. Such a synthetic procedure could provide access to a broad and structurally diverse group of candidate compounds suitable for biological testing.

#### *N*,*N*-Dialkyl-*N'*-Chlorosulfonylchloroformamidines in Heterocyclic Synthesis. II. Thiazolo-, Thiadiazolo-, and Oxadiazolo-Fused [1,2,4,6]-Thiatriazine Dioxides

Gary D. Fallon, Craig L. Francis, Katarina Johansson, Andris J. Liepa, Ruth C. J. Woodgate

*N*,*N*-dialkyl-*N'*-chlorosulfonylchloroformamidines **1** are versatile 1,3-dielectrophilic intermediates for the synthesis of new heterocycles. This paper reports the preparation and full characterization of a series of novel, fused [1,2,4,6]thiatriazine dioxides (such as **2** and **3**) via the reaction of **1** with several 2-amino-1-azaheterocycles.

Aust. J. Chem. 2005, 58, 891-900.

#### Quaternary Ammonium Arylspiroborate Esters as Organo-Soluble, Environmentally Benign Wood Protectants

Jenny M. Carr, Peter J. Duggan, David G. Humphrey, James A. Platts, Edward M. Tyndall

Aust. J. Chem. 2005, 58, 901-911.

# Wood treated with (2) +N(nBu)4 Untreated wood

With currently used wood preservatives facing a demise due to their less than environmentally friendly nature, the search is on for viable alternatives. 'Green' boron-based wood preservatives are currently being developed as replacements. Here the anti-fungal and termiticidal activities, and the resistance to leaching from timber, of three related tetra-*n*-buylammonium spiroborates have been examined.

# Two New Biocatalysts for Improved Biological Oxidation of 1,8-Cineole

Jo-Anne M. Rasmussen, Kylie A. Henderson, Melissa J. Straffon, Geoffrey J. Dumsday, Jacqueline Coulton, Michael Zachariou

Aust. J. Chem. 2005, 58, 912-916.

Biocatalysis is limited by the very few commercially available biocatalysts. Here we report two new biocatalysts (one fungal, one bacterial) for the oxidation of a model bicyclic terpene. These biocatalysts show improved tolerance to the terpene as well as improved yields of the oxidized products.

**Annual Author Index** p. 917