

# AUSTRALIAN JOURNAL OF CHEMISTRY

AN INTERNATIONAL JOURNAL FOR CHEMICAL SCIENCE

## RESEARCH FRONT: Ionic Liquids – Latest Advances

### Foreword

#### The 3rd Australasian Symposium on Ionic Liquids (ASIL-3)

Jennifer M. Pringle

*Aust. J. Chem.* **2009**, 62, 287.



This special issue features a collection of papers presented at the 3rd Australasian Symposium on Ionic Liquids, held in Melbourne in 2008. The breadth of topics reflects the widespread applicability of ionic liquids, and the papers chosen demonstrate some of the key research areas in the field.

### Reviews

#### Correlations in the Structure and Dynamics of Ionic Liquids

Angus Gray-Weale

*Aust. J. Chem.* **2009**, 62, 288–297.

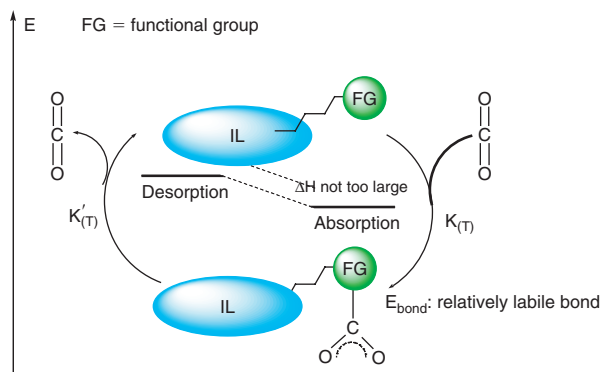
I explore the use of modern computational methods to guide or aid laboratory work on ionic liquids, and the importance of ‘old-fashioned’ theory, from before the age of fast computers. Most simulations of ionic liquids to date have used ‘atomistic’ methods, and I argue for an alternative approach to understanding transport processes.

#### Why are Ionic Liquids Attractive for CO<sub>2</sub> Absorption? An Overview

Junhua Huang, Thomas Rüther

*Aust. J. Chem.* **2009**, 62, 298–308.

In (re)search for powerful materials for the efficient removal of CO<sub>2</sub> from green-house gas emission, there is considerable interest in ionic liquids (ILs) as new CO<sub>2</sub> absorbents. This paper evaluates the advantages and disadvantages of ILs, and provides an overview of the recent developments of ILs for CO<sub>2</sub> capture.

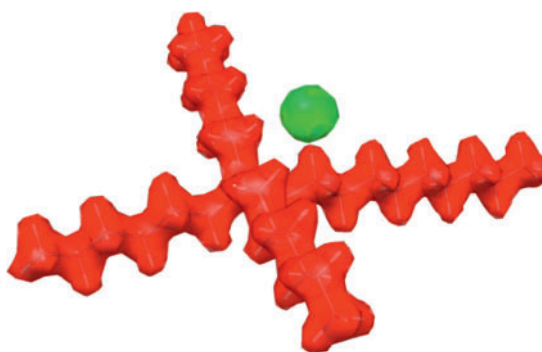


## Phosphonium-Based Ionic Liquids: An Overview

Kevin J. Fraser,  
Douglas R. MacFarlane

*Aust. J. Chem.* **2009**, 62, 309–321.

Phosphonium cation-based ionic liquids (ILs) are a readily available family of ILs that in some applications offer superior properties as compared to nitrogen cation-based ILs. Here, the authors provide an overview of the properties of these interesting materials and the applications in which they are appearing.



## Rapid Communication

### An Efficient and Simple One-Pot Synthesis of $\beta$ -Acetamido Ketones Catalyzed by Ytterbium Triflate in Ionic Liquid

Anil Kumar, M. Sudershan Rao,  
Israr Ahmad, Bharti Khungar

*Aust. J. Chem.* **2009**, 62, 322–327.

In this study  $\text{Yb}(\text{OTf})_3$  was immobilized in ionic liquid and shown to be an effective and reusable catalyst for one-pot synthesis of  $\beta$ -acetamido ketones by three-component coupling at room temperature. Simplicity, good yield of products, efficiency and reusability of the catalyst, and clean reaction conditions are the salient features of this method.

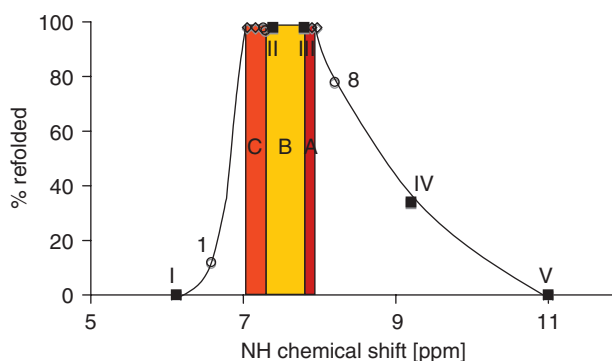
## Full Papers

### The ‘Refoldability’ of Selected Proteins in Ionic Liquids as a Stabilization Criterion, Leading to a Conjecture on Biogenesis

Nolene Byrne, Jean-Philippe Belieres, C. Austen Angell

*Aust. J. Chem.* **2009**, 62, 328–333.

Protein folding is studied in solution environments that are very different from the usual aqueous buffers in order to understand why hydrated protic ionic liquids (pILs) should be so hospitable to biomolecules. The ability of common hydrophilic proteins in these media to withstand repeated unfoldings with little protein loss is quantified by a refolding index (RFI) based on calorimetric scans, and high RFI composition zones are identified for two common proteins. Similar results are then identified in ‘primitive’ (ammonium salt) pILs, and this leads to a conjecture aimed at resolving the hydrolysis problem faced by conventional ‘primordial soup’ theories of abiogenesis.

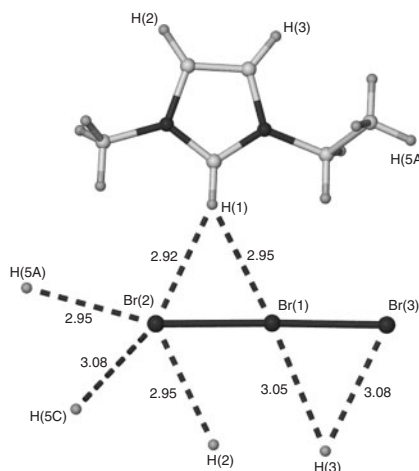


### Structural Characterization of Novel Ionic Salts Incorporating Trihalide Anions

Pamela M. Dean, Bronya R. Clare, Vanessa Armel, Jennifer M. Pringle, Craig M. Forsyth, Maria Forsyth, Douglas R. MacFarlane

*Aust. J. Chem.* 2009, **62**, 334–340.

Here we report the first crystal structure analysis of low melting salts utilising trihalide anions in combination with typical ionic liquid (IL) organic cations namely, 1-ethyl-3-methylimidazolium tribromide ( $[\text{C}_2\text{mim}][\text{Br}_3]$ ), 1-ethyl-1-methylpyrrolidinium tribromide ( $[\text{C}_2\text{mpyr}][\text{Br}_3]$ ) and 1-propyl-1-methylpyrrolidinium triiodide ( $[\text{C}_3\text{mpyr}][\text{I}_3]$ ). The interactions between the anion and cation of the salt are of significant interest since distinctive properties ascribed to ionic liquids are determined to a certain extent by these interactions.



### Processing of Electric Arc Furnace Dust using Deep Eutectic Solvents

Andrew P. Abbott, John Collins, Ian Dalrymple, Robert C. Harris, Reena Mistry, Fulian Qiu, James Scheirer, William R. Wise

*Aust. J. Chem.* 2009, **62**, 341–347.

Electric arc furnace dust is a widely produced waste material from the steel-making industry. This paper shows a novel process that can take a complex mixture of heavy metals and separate them into a valuable source of important raw materials. The process uses environmentally compatible solvents for the extraction and separation.

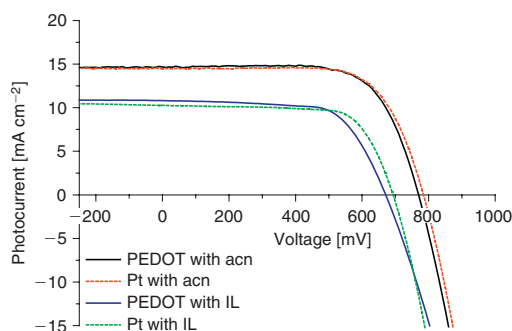


### PEDOT-Coated Counter Electrodes for Dye-Sensitized Solar Cells

Jennifer M. Pringle, Vanessa Armel, Maria Forsyth, Douglas R. MacFarlane

*Aust. J. Chem.* 2009, **62**, 348–352.

Platinum is one of the most expensive components of dye-sensitized solar cells (DSSCs) and its high temperature deposition is problematic for bulk scale synthesis and use of plastic substrates. Poly(3,4-ethylenedioxythiophene) (PEDOT)-coated counter electrodes for DSSCs have been prepared at ambient temperature and without the use of iron-based oxidants. These show a comparable electrocatalytic performance to conventional Pt counter electrodes, with solar cell efficiencies >7.5%.



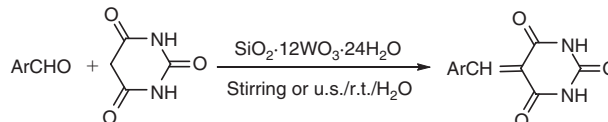
## Rapid Communications

**SiO<sub>2</sub>·12WO<sub>3</sub>·24H<sub>2</sub>O: a Highly Efficient Catalyst for the Synthesis of 5-Arylidene Barbituric Acid in the Presence of Water**

Ji-Tai Li, Ming-Xuan Sun

*Aust. J. Chem.* **2009**, 62, 353–355.

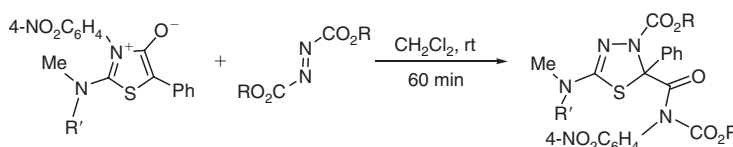
The development of new catalysts for carbon–carbon bond formation in aqueous media is an increasingly important objective. The environmentally friendly catalyst, silicotungstic acid, offers high catalytic activity and good stability. The preparation of a range of 5-arylidene barbituric acids catalyzed by silicotungstic acid was carried out in high yield in the presence of water at room temperature.

**Facile Synthesis of 4,5-Dihydro-1,3,4-Thiadiazoles by 1,3-Dipolar Cycloaddition of Thioisomünchnones**

Bárbara Sánchez, José Luis Bravo, María José Arévalo, Ignacio López, Mark E. Light, Guadalupe Silvero

*Aust. J. Chem.* **2009**, 62, 356–359.

Thiadiazoles constitute an important family of compounds due to their potential biological effects, such as anti-tumour, antibacterial, anti-inflammatory, and pesticide action. This article presents a novel method for obtaining a type of 1,3,4-thiadiazoles by means of the 1,3-cycloaddition of thioisomünchnones with azodipolarophiles.



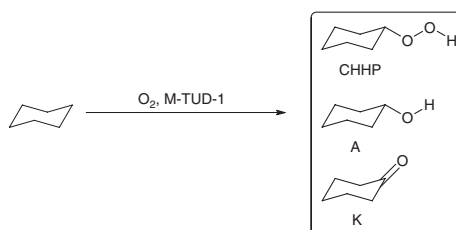
## Full Papers

**Metal-TUD-1 Catalyzed Aerobic Oxidation of Cyclohexane: A Comparative Study**

Ramanathan Anand, Mohamed S. Hamdy, Rudy Parton, Thomas Maschmeyer, Jacobus C. Jansen, Roger Gläser, Freek Kapteijn, Ulf Hanefeld

*Aust. J. Chem.* **2009**, 62, 360–365.

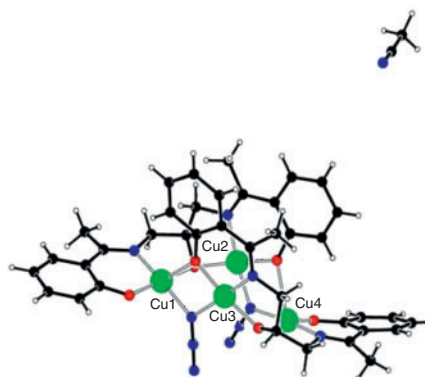
Various metal-incorporated, TUD-1 structure-type, mesoporous silicas have been evaluated for the selective aerobic oxidation of cyclohexane with *tert*-butylhydroperoxide and cyclohexylhydroperoxide (CHHP). The formation of the respective hydroperoxides and subsequent decomposition to the alcohol and ketone is reported. Judicious selection of metal and metal loading may tune the catalyst for either CHHP formation or CHHP decomposition.

**A Novel  $\mu_{1,1}$ -Azido-,  $\mu_2$ -Alkoxo-, and  $\mu_2$ -Phenoxo-Bridged Tetranuclear Copper(II) Complex with a Quinquedentate Schiff-Base Ligand: Magneto-Structural and DFT Studies**

Subhra Basak, Soma Sen, Georgina Rosair, Cédric Desplanches, Eugenio Garribba, Samiran Mitra

*Aust. J. Chem.* **2009**, 62, 366–375.

A novel tetranuclear complex [Cu<sub>4</sub>L<sub>2</sub>( $\mu_{1,1}$ -N<sub>3</sub>)<sub>2</sub>]·CH<sub>3</sub>CN has been synthesized using a N<sub>2</sub>O<sub>3</sub>-donor Schiff-base ligand **H<sub>3</sub>L** (*N,N'*-(2-hydroxypropane-1,3-diyl)bis(2-hydroxyacetophenimine)) and characterized. X-ray single-crystal structure reveals three kinds of bridges among the four metal centres: one from the exogenous azido ligand and two from the phenoxo and alkoxo moieties of **H<sub>3</sub>L**. Variable-temperature magnetic susceptibility measurements and density functional theory calculations confirm that the antiferromagnetic effect through the alkoxo-bridged Cu<sup>II</sup> centres combined with the ferromagnetic interaction through the azido-bridged metal centres results in an *S* = 0 ground state.

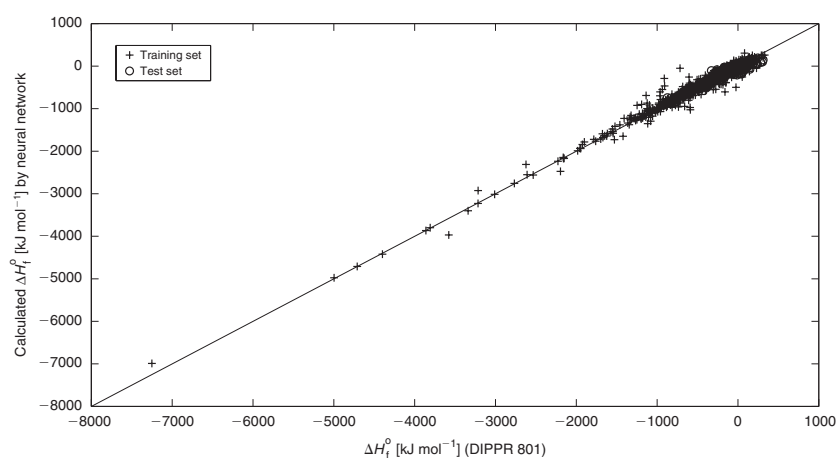


## Prediction of the Standard Enthalpy of Formation of Pure Compounds Using Molecular Structure

Farhad Gharagheizi

*Aust. J. Chem.* **2009**, 62, 376–381.

A new molecular structure-based model for the prediction of the standard enthalpy of formation of pure compounds is presented. Having been used to confirm  $\Delta H_f^\circ$  of 1692 pure compounds that belong to many chemical families, this is the most comprehensive model presented for the prediction of  $\Delta H_f^\circ$  of pure compounds so far.

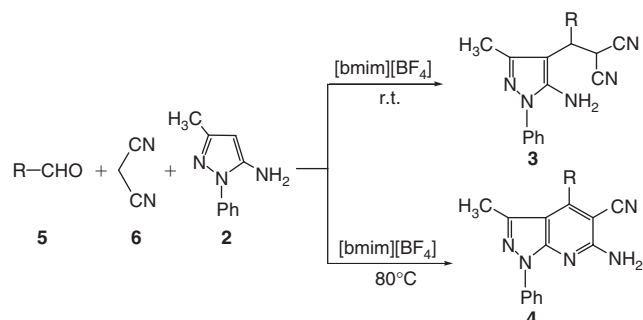


## Controllable Synthesis of Pyrazolo[3,4-*b*]pyridines or Substituted Malononitrile Derivatives through Multi-Component Reactions in Ionic Liquid

Xinying Zhang, Xiaoyan Li,  
Xuesen Fan, Xia Wang,  
Jianji Wang, Guirong Qu

*Aust. J. Chem.* **2009**, 62, 382–388.

Ionic liquid technology offers a new and environmentally benign approach toward organic synthesis. A convenient, efficient, and controllable synthesis of two series of heterocyclic products in an ionic liquid is described herein. The methods can be transferred to other Knoevenagel-type condensations and may be developed as a novel alternative for the preparation of N-heterocycles.

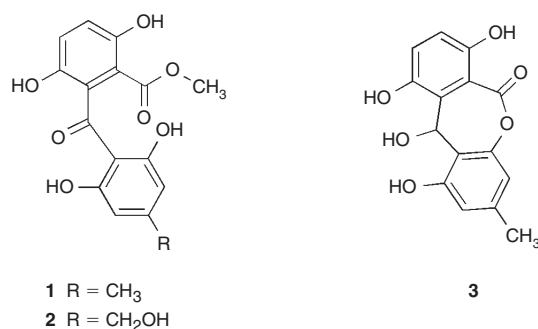


## Graphisins A and B from the Lichen *Graphis tetralocularis*

Pattama Pittayakhajonwut,  
Veera Sri-indrasutdhi,  
Aibrohim Dramaee, Sanisa Lapanun,  
Rapheephath Suvannakad,  
Morakot Tantichareon

*Aust. J. Chem.* **2009**, 62, 389–391.

The observed anti-tuberculosis activity of the crude extracts of the lichen *Graphis tetralocularis* has led to the isolation of acremonidin E (**1**) and graphisins A (**2**) and B (**3**). The biological activity of the isolated compounds against *Mycobacterium tuberculosis* and their cytotoxicity against cancerous and non-cancerous cells are evaluated.



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Corrigendum

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**Microwave-Assisted Tandem  
Processes for the Synthesis of  
N-Heterocycles (appearing in  
*Aust. J. Chem.* 2009, 62, 208–222)**

*Mohammed Abid, Béla Török,  
Xudong Huang*

*Aust. J. Chem.* **2009**, 62, 392.

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