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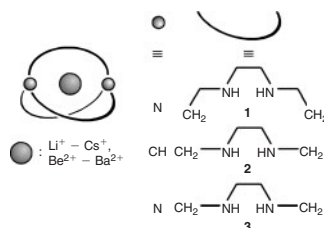
AN INTERNATIONAL JOURNAL FOR CHEMICAL SCIENCE

Full Papers

Host–Guest Complexes of Bicyclic Hexamine Cryptands – Prediction of Ion Selectivity by Quantum Chemical Calculations. III

Ralph Puchta, Roland Meier,
Rudi van Eldik

Aust. J. Chem. **2007**, *60*, 889–897.



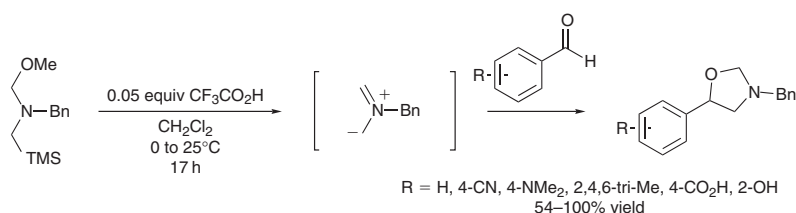
Quantum chemical investigations of cryptands **1**, **2**, and **3** predict a favourable binding of K^+ and Ba^{2+} in **1**, and binding of Li^+ and Mg^{2+} by **2** and **3**. To facilitate the best coordination mode, the cryptands have to fold around the cations by twisting their torsion angles. Therefore, the investigated cryptands could be alternatives to the well-known cryptands [2.2.2] and [2.1.1].

Synthesis of 5-Aryloxazolidines via 1,3-Dipolar Cycloaddition Reaction of a Non-Stabilized Azomethine Ylide with Aromatic Aldehydes

John H. Ryan, Nadia Spiccia,
Leon S.-M. Wong, Andrew B. Holmes

Aust. J. Chem. **2007**, *60*, 898–904.

The 1,3-dipolar cycloaddition of an azomethine ylide with an aromatic aldehyde produces the biologically significant 5-aryloxazolidine core. A range of aromatic and heteroaromatic aldehydes were explored and generally high yields of 5-aryloxazolidines were obtained. Low conversions and side reactions were observed for certain phenolic and pyrrolic aldehydes.



Synthesis of 4-Aryl-3(5)-(2-hydroxyphenyl)pyrazoles by Reaction of Isoflavones and their 4-Thio Analogues with Hydrazine Derivatives

Albert Lévai, Artur M. S. Silva,
José A. S. Cavaleiro, José Elguero,
Ibon Alkorta, József Jekő

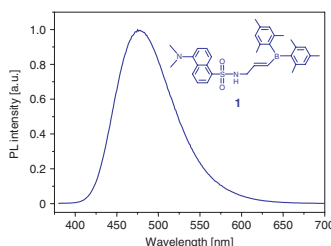
Aust. J. Chem. **2007**, *60*, 905–914.

New potential pharmacological 4-aryl-3(5)-2-(hydroxyphenyl)pyrazoles have been prepared by the reaction of isoflavones and their 4-thio analogues with hydrazines. The reaction mechanism for the formation of these pyrazoles is discussed, and the new compounds have been fully characterized by NMR spectroscopy. The tautomeric behaviour of the obtained compounds was investigated by NMR spectroscopy and theoretical calculations.

Fluorescent Ethenyl- and Ethynyl-dimesitylboranes Derived from 5-(Dimethylamino)-N-(prop-2-ynyl)naphthalene-1-sulfonamide

Wai-Yeung Wong, Suk-Yue Poon,
Mei-Fang Lin, Wai-Kwok Wong

Aust. J. Chem. **2007**, *60*, 915–922.

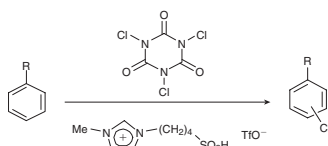


New fluorescent dimesitylvinylborane **1** and dimesitylethynylborane **2**, which contain the dansyl chromophore, have been synthesized. Their spectroscopic, photophysical, electrochemical, and structural properties have been studied in detail. The electroluminescence behaviour of **1** in multilayered organic light-emitting diodes showed blue-light emission with moderate device efficiency in a doped guest–host system.

Chlorination of Aromatics with Trichloroisocyanuric Acid (TCICA) in Brønsted-Acidic Imidazolium Ionic Liquid [BMIM(SO₃H)][OTf]: an Economical, Green Protocol for the Synthesis of Chloroarenes

Abigail Hubbard, Takao Okazaki,
Kenneth K. Laali

Aust. J. Chem. **2007**, 60, 923–927.

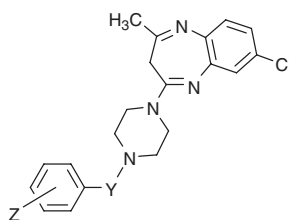


An economical, green, method for the synthesis of chloroarenes under mild conditions is described. The imidazolium-based Brønsted acidic ionic liquid [BMIM(SO₃H)][OTf] is employed as catalyst and solvent, and trichloroisocyanuric acid (TCICA) as chlorinating agent. Mild conditions, facile recovery and recycling of the ionic liquid, a simple product isolation step, and the use of TCICA as a readily available, cheap, chlorinating agent are some of the positive attributes of this method, which avoids the use of chlorine gas and/or strong/corrosive acids.

Synthesis and Preliminary Pharmacological Evaluation of 4'-Arylalkyl Analogues of Clozapine. III. Replacement of the Tricyclic Nucleus with a Bicyclic Template

Ben Capuano, Ian T. Crosby,
Edward J. Lloyd, David A. Taylor

Aust. J. Chem. **2007**, 60, 928–933.

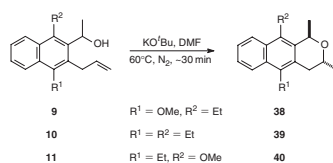


The synthesis of a 'next generation' of bicyclic analogues of clozapine, based on a modification of the structural hybridization of the antipsychotics haloperidol and clozapine, is reported. The study investigates the biochemical effects of some aryl substituents (Z) and the length and nature of the linker (Y) (see structure). The results of preliminary pharmacological studies are also presented.

Naphthopyrans and their C4 Alcohols by Cyclization of Substituted Naphthalenes using Potassium *t*-Butoxide in Dimethylformamide. Generality and Stereochemical, including Conformational, Effects

Robin G. F. Giles, Ivan R. Green,
Wendell P. Swigelaar, C. Peter Taylor

Aust. J. Chem. **2007**, 60, 934–945.

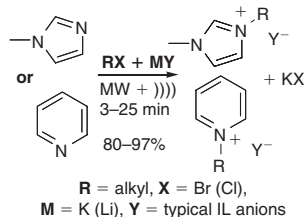


An understanding of methods for the construction of naphthopyrans is important because a significant number of their members show an array of biological activities and they are also of potential medicinal value. The present paper establishes the breadth of a remarkable method for the assembly of some of these compounds. If any of these compounds are found to be important, this method will facilitate their acquisition through its high yields and selectivity.

A Speedy One-Pot Synthesis of Second-Generation Ionic Liquids Under Ultrasound and/or Microwave Irradiation

Giancarlo Cravotto, Luisa Boffa,
Jean-Marc L'evêque, Julien Estager,
Micheline Draye, Werner Bonrath

Aust. J. Chem. **2007**, 60, 946–950.



Both microwave heating and power ultrasound are being increasingly exploited in organic synthesis, and their combined use is one of the most promising innovations. These techniques pave the road for straightforward access to a wide range of room-temperature ionic liquids, dramatically reducing preparation times and costs. The most common ionic liquids that are finding a growing wealth of chemical applications can be prepared on a laboratory scale in a few minutes and high yields.

Photoassisted Catalytic Cleavage of the C–F Bond in Pentafluorophenol With ZnO and the Effect of Operational Parameters

Lakshiminarasimhan Ravichandran,
Kaliyamoorthy Selvam,
Meenakshisundaram Swaminathan

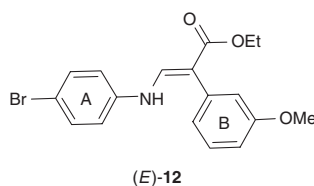
Aust. J. Chem. **2007**, 60, 951–956.

Mineralization of toxic pentafluorophenol with an eco-friendly photocatalyst, zinc oxide, is reported. Addition of oxidants and metal ions enhances the efficiency of zinc oxide. The defluorination with zinc oxide was more effective at 254 nm than at 365 nm UV light.

Synthesis and Structure–Activity Relationship Analysis of Enamines as Potential Antibacterial Agents

Jia-Yu Xue, Zhu-Ping Xiao, Lei Shi,
Shu-Hua Tan, Huan-Qiu Li,
Hai-Liang Zhu

Aust. J. Chem. **2007**, *60*, 957–962.



Enamines are similar in their chemical structure to Schiff bases, compounds that have been widely studied for biological applications. Here 24 novel enamines are synthesized and their inhibitory effects against a range of bacteria and fungi are investigated. Structure–activity relationship analyses reveal that (*E*)-enamines generally exhibit higher antibacterial activity than the corresponding (*Z*)-isomers.

Focus

The Bestmann–Ohira Reagent for the Conversion of Aldehydes into Terminal Alkynes

Shannon D. Zannatta

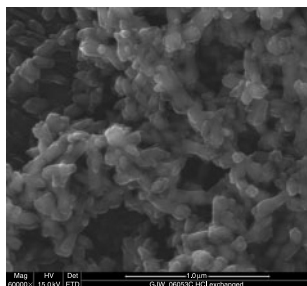
Aust. J. Chem. **2007**, *60*, 963.

Terminal alkynes are extremely useful functional groups in many organic transformations. The easy-to-prepare Bestmann–Ohira reagent, allows the mild and efficient transformation of aldehydes to terminal alkynes. This chemoselective reagent has been used in a wide range of applications from simple functional group conversions to complex natural product syntheses.

Solvothermal Synthesis of Nanostructured Energy Storage Materials

Gregory J. Wilson

Aust. J. Chem. **2007**, *60*, 964.



The use of solvothermal methods as an inexpensive and environmentally benign manner to produce nanostructured materials for energy storage applications is discussed. The effect of structure and morphology is presented as a means of controlling physical properties and the implication these have on charge and discharge kinetics for Li-ion or H⁺ redox processes. Solvothermal synthesis is presented as an effective means of producing nanostructured metal oxides for high-rate energy storage applications such as asymmetric supercapacitors and batteries.