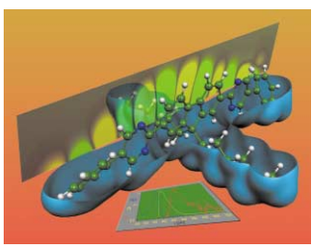
ISSN 1477–0520 OBCRAK(17) 2999–3138(2003)

Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica



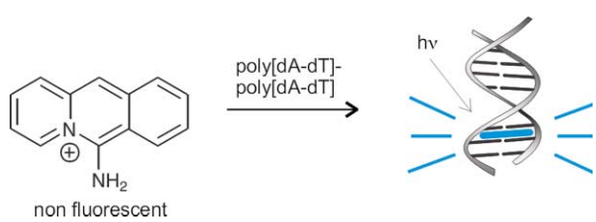
Cover

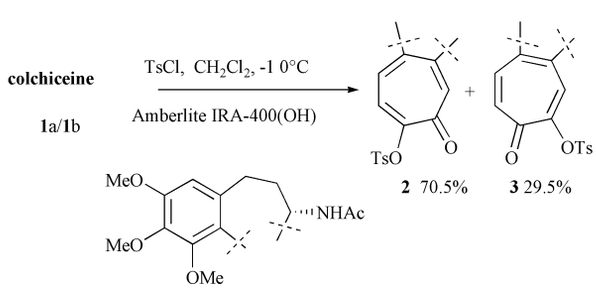
See G. Hughes, C. Wang, A. S. Batsanov, M. Fern, S. Frank, M. R. Bryce, I. F. Perepichka, A. P. Monkman and B. P. Lyons, page 3069.

The structure of 2,7-bis(5-phenyl-2-pyrimidyl)-9,9-dihexylfluorene, which has been used as the emissive layer in an organic light-emitting diode. Both experimental and computational data indicate that incorporation of the 2-pyrimidine moiety into the oligoarylene backbone facilitates the planarisation of this fragment and permits a degree of control over the HOMO/LUMO energy levels.

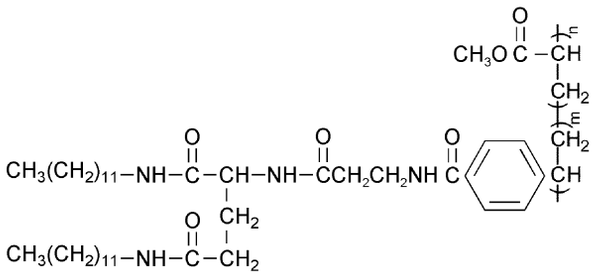
contents

COMMUNICATIONS





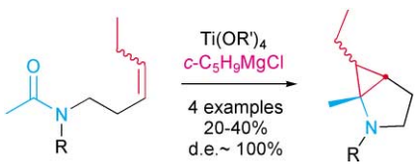
COMMUNICATIONS



Novel self-assembling organogelators by combination of a double chain-alkylated L-glutamide and a polymeric head group

Hirotaka Ihara, Makoto Takafuji, Toshihiko Sakurai, Masahiro Katsumoto, Noriko Ushijima, Tomohiro Shirosaki and Hiroshi Hachisako

We report on a new class of L-glutamide-derived organogelators with polymeric head groups and a molecular design which facilitates the addition of specific functionality. We expect this new class to expand possible applications of organogelators.

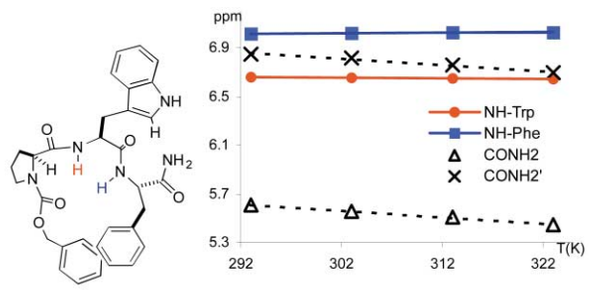


Studies on the intramolecular Kulinkovich–de Meijere reaction of disubstituted alkenes bearing carboxylic amide groups

Nouara Ouhamou and Yvan Six

1,2-Disubstituted olefins bearing an acetamide group undergo intramolecular Kulinkovich–de Meijere cyclopropanation in moderate yield but almost complete diastereoselectivity.

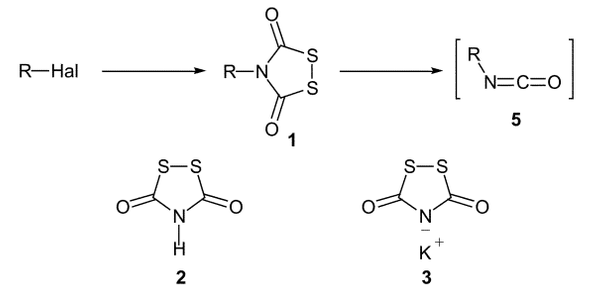
ARTICLES



Conformational analysis and μ-opioid receptor affinity of short peptides, endomorphin models in a low polarity solvent

Giuliana Cardillo, Luca Gentilucci, Alessandra Tolomelli, Ahmed R. Qasem, Santi Spampinato and Maria Calienni

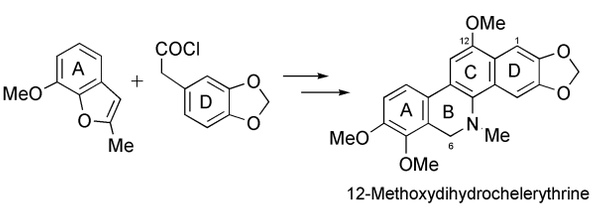
The carbamate-peptide Cbz-Pro-Trp-PheNH_2 shows a nanomolar affinity for μ-opioid receptors, and adopts a compact conformation in $CDCl_3$, stabilized by intramolecular H-bonds.



Synthetic and structural studies on 1,2,4-dithiazolidine-3,5-dione derivatives

Mark E. Wood, Daniel J. Cane-Honeysett, Michael D. Dowle, Simon J. Coles and Michael B. Hursthouse

Methods have been developed for the direct *N*-alkylation of 1,2,4-dithiazolidine-3,5-dione **2** and the conversion of the products **1** into isocyanates **5**. X-ray crystallographic data are presented for potassium 1,2,4-dithiazolidine-3,5-dione **3**.



Total synthesis of 12-methoxydihydrochelerythrine and anti-tumour activity of its quaternary base: toward an efficient synthetic route for 12-alkoxybenzo[*c*]phenanthridine bases *via* naphthoquinone monooxime from 2-benzofuranyl-1-tetralone derivative

Toshiko Watanabe, Yoshiaki Ohashi, Rie Yoshino, Naoko Komano, Miyuki Eguchi, Sakiko Maruyama and Tsutomu Ishikawa

A concise total synthesis of 12-methoxydihydrochelerythrine from a benzofuran *via* naphthoquinone monooxime is described.

RSC **Journals Archive**

RS•C

advancing the chemical sciences

For many reasons (including library space, degeneration of paper issues and the wider availability of data), there is an increasing demand for electronic access (including searching capability) to all chemical research previously published by the RSC. To meet this demand, we are pleased to announce that the RSC Journals Archive Project is underway.

- The archive will contain all articles published by the Royal Society of Chemistry (and its forerunner societies) from 1841 to 1996. It is estimated the archive will contain 210,000 articles in 1,200,000 pages. The project will be completed during the course of this year, and the archive will be available from the beginning of 2004.
- The articles will be available via issue contents lists and by full-text searches of the articles. A Digital Object Identifier (DOI) will be assigned to each article.
- In addition, the references in the 1990-1996 articles will contain "reference links" to full text and CAS abstracts, where available.

The purchase options for a single site will be as follows:

Outright purchase *(RSC-hosts)*
£25,000 / $40,000*
plus annual maintenance fee:
£500 / $800
Outright purchase *(customer-hosts)*
£25,000 / $40,000*
Annual lease
£1,500 / $2,400
Outright purchase *(over two years)*
£30,000 / $48,000*
Package A-Plus
See www.rsc.org/archive for details
**Package A subscribers will be given a 10% discount.*

Prices are subject to local tax, where applicable.

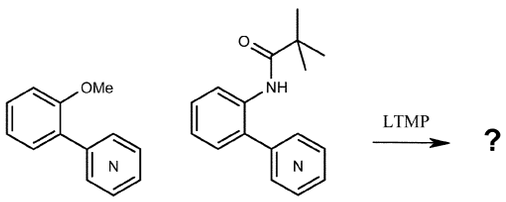
For consortium and multi-site access, please contact the RSC for pricing.

To enable us to keep you abreast of how the RSC Journals Archive Project is progressing, please register your name for e-alerts via the URL below:

www.rsc.org/archive

RSCAD/10070303-COLOUR

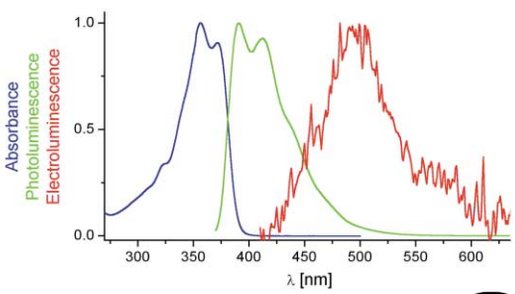
Orders & further details · Ms Lesley Maw · Sales & Customer Care Dept · Royal Society of Chemistry
Thomas Graham House · Science Park · Milton Road · Cambridge · CB4 0WF · UK
T +44(0)1223 432360 · F +44(0)1223 426017 · E sales@rsc.org
Or visit our websites: www.rsc.org and www.chemsoc.org
Registered Charity No. 207890



Synthesis and deprotonation of 2-(pyridyl)phenols and 2-(pyridyl)anilines

Anne-Sophie Rebstock, Florence Mongin, François Trécourt and Guy Quéguiner

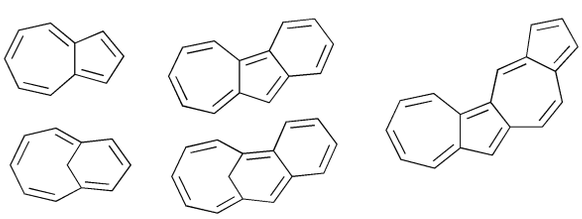
When treated with LTMP, nitrogen- and oxygen-based (2-substituted phenyl)pyridines were deprotonated.



New pyrimidine- and fluorene-containing oligo(arylene)s: synthesis, crystal structures, optoelectronic properties and a theoretical study

Gregory Hughes, Changsheng Wang, Andrei S. Batsanov, Michael Fern, Stephen Frank, Martin R. Bryce, Igor F. Perepichka, Andrew P. Monkman and Benjamin P. Lyons

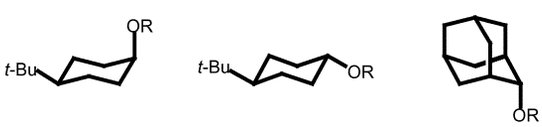
Compound **16** has been used as the emissive layer in an OLED: at a high turn-on voltage blue-green light (λ_{max} 500 nm) is emitted which most likely emanates primarily from excimer states.



A theoretical (DFT, GIAO-NMR, NICS) study of the carbocations and oxidation dications from azulenes, homoazulene, benzazulenes, benzohomoazulenes, and the isomeric azulenoazulenes

Takao Okazaki and Kenneth K. Laali

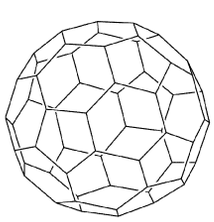
Carbocations and oxidation dications derived from a series of azulene-based hydrocarbons were studied by DFT calculations.



Low-temperature X-ray structural studies of the ester and ether derivatives of *cis*- and *trans*-4-*tert*-butyl cyclohexanol and 2-adamantanol: application of the *variable oxygen probe* to determine the relative σ-donor ability of C–H and C–C bonds

Marisa Spiniello and Jonathan M. White

The *variable oxygen probe* approach is applied to three series of low temperature X-ray structures and this technique suggests little relative difference in the σ-donor ability of C–H and C–C bonds.



CF_3CO_2Ag

300 °C,
0.05 mBar

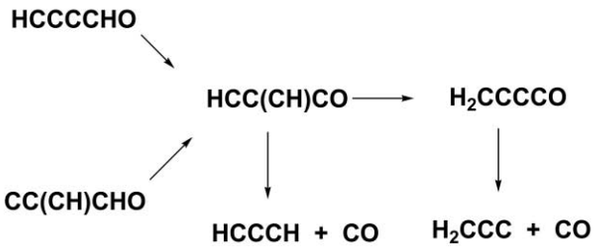
$[C_{60}(CF_3)_n]_m$

n	*m*
2	1
4	8
6	13
8	21
10	11
12	5
14	4

Unusual addition patterns in trifluoromethylation of [60]fullerene

Adam D. Darwish, Ala'a K. Abdul-Sada, Anthony G. Avent, Yury Lyakhovetsky, Elena A. Shilova and Roger Taylor

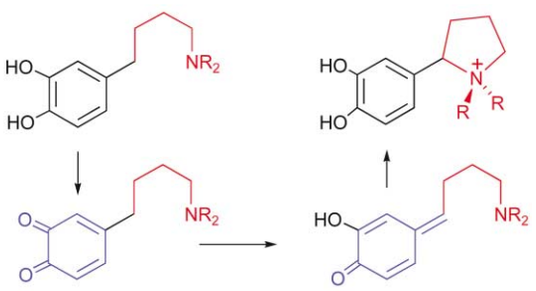
Trifluoromethylation of [60]fullerene produces more derivatives and isomers than any other reaction but no dominant product. Kinetic control may therefore be important in this reaction.



Gas phase generation of the neutrals H_2CCCCO, HCCCCDO and CCCHCHO from anionic precursors. Rearrangements of HCCCCDO and CCCHCHO. A joint experimental and theoretical study

Mark Fitzgerald, John H. Bowie and Suresh Dua

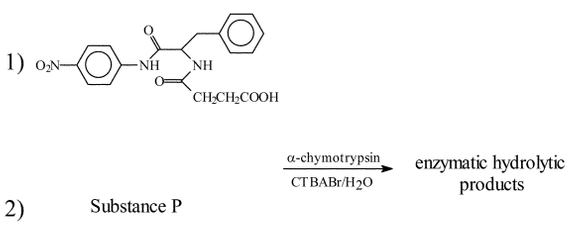
Isomers H_2CCCCO and HCCCCHO have been formed from precursor anions: energised HCCCCHO rearranges to H_2CCCCO.



Formation of *para*-quinomethanes *via* 4-aminobutylcatechol oxidation and *ortho*-quinone tautomerism

Edward J. Land, Christopher A. Ramsden, Patrick A. Riley and Gnanamoly Yoganathan

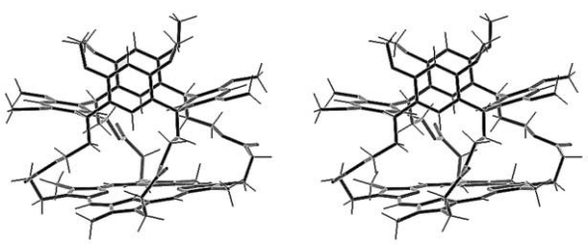
4-(4-*N*,*N*-Dialkylaminobutyl)catechols are oxidised chemically and enzymatically to *N*,*N*-dialkylpyrrolidinium salts *via* *ortho*-quinone and *para*-quinomethane intermediates.



ESI-MS in the study of the activity of α-chymotrypsin in aqueous surfactant media

Francesco De Angelis, Alessandra Di Tullio, Piero Del Boccio, Samantha Reale, Gianfranco Savelli and Nicoletta Spreti

ESI-MS has been used to investigate α-chymotrypsin activity in aqueous surfactant solutions, also towards substrates not amenable to UV-Vis detection.



Synthesis and molecular modelling studies of resorcin[4]arene-capped porphyrins

Bruno Botta, Paola Ricciardi, Carlo Galeffi, Maurizio Botta, Andrea Tafi, Rebecca Pogni, Rosa Iacovino, Isidoro Garella, Benedetto Di Blasio and Giuliano Delle Monache

Three new resorcin[4]arene-capped porphyrins (**3**, **5** and **7**) different in the porphyrin skeleton, in the linking arms and in the cavity dimensions, have been synthesised.

Dates, venues and contact details of forthcoming events.

* Indicates the author for correspondence: see article for details.

Electronic supplementary information is available on http://www.rsc.org/esi: see article for further information.