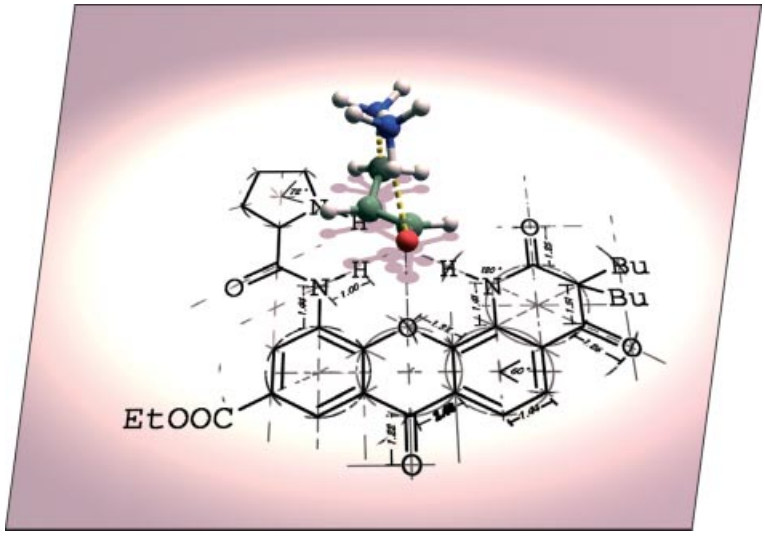
The EUChemSoc Societies have taken the significant step into the future by merging their traditional journals, to form two leading chemistry journals, the *European Journal of Inorganic Chemistry* and the *European Journal of Organic Chemistry*. Three further EUChemSoc Societies (Austria, Czech Republic and Sweden) are Associates of the two journals.

COVER PICTURE

The cover picture shows the design of molecular receptors with enzyme-like catalytic activity for the Michael addition of pyrrolidine to an α,β-unsaturated lactam. The picture emphasizes the design process of these receptors by using a draft-like style for the receptor structure. This design is based on a model for the transition state (represented as a high-quality 3-D model) that is obtained from theoretical study of the reaction mechanism. In the paper, we use both kinetic experiments and molecular modeling studies to assist the design of the H-bonding catalyst. From these studies we concluded that the presence of an auxiliary amine group could improve the catalytic activity of previous catalysts that resemble the oxyanion hole structure found in many enzymes. A simple modeling procedure is used to predict the catalytic activity of the tested catalyst, that in some cases shows k_{cat}/k_{uncat} values close to the range of values observed for many catalytic antibodies. Details are discussed in the article by L. Simón et al. on p. 4821ff.



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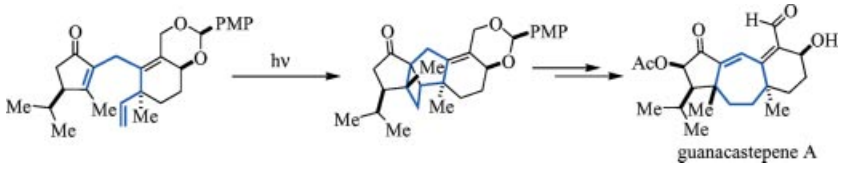
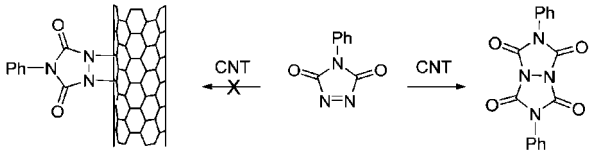
MICROREVIEW



The application of photocycloaddition to natural product synthesis continues to produce innovative strategies for key bond constructions in the complex molecule environment. This Microreview surveys the recent literature for photocycloaddition key steps in natural product synthesis, examining both completed routes and those in progress.

SHORT COMMUNICATION

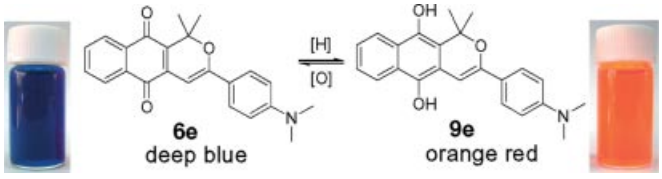


The reactivity of triazolinedione (TAD) was investigated in the Diels–Alder reaction with carbon nanotubes. However, an unexpected conversion of TAD into its dimer was observed. ESR spectroscopy suggested that the process was initiated by electron transfer from the nanotubes.

FULL PAPERS

The theozyme concept has been used in the design of artificial enzymes that show k_{cat}/k_{uncat} values of up to 10^4 in Michael addition reactions of pyrrolidine to α,β-unsaturated lactams. The receptors combine "oxyanion hole" structures with amino groups responsible for the proton transport of the nucleophile. Computational chemistry applications in the catalyst design are also investigated.

Redox Switches

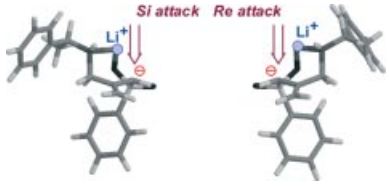


Trisubstituted naphthopyrandione derivatives were prepared; quinone **6e** instantly changed from deep blue to orange red when treated with $NaBH_4$ in MeOH. Hydroquinone **9e** reverted back to its original color when the reducing agent was removed. Quinone **6e** did not show fluorescence prior to reduction, but hydroquinone **9e** emitted red fluorescence.

Keywords: Quinones / Redox chemistry / Fluorescence / Donor–acceptor systems

Stereoselectivity and Li Anions

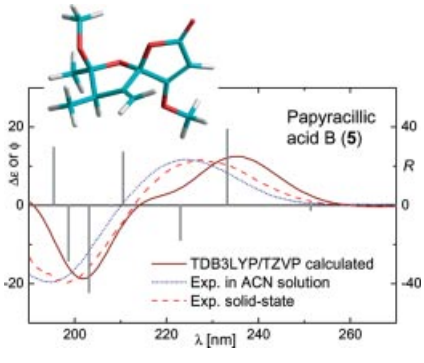
Qualitative modeling indicates that the observed stereoselectivity in Michael additions is due to steric requirements of the reagents at VDW distances, Ph–Li^+ bonding in the carbanion, and electrostatic factors.



Keywords: Michael addition / Carbanions / Diastereoselectivity / Conformational analysis

Fungal Metabolites

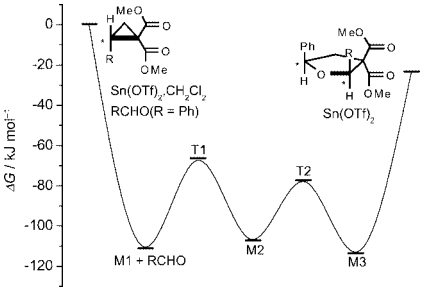
Five new metabolites, palmarumycin M_1 (**1a**) and M_2 (**3**), papyracillic acid C (**6**) and the microsphaeropsins A (**7**) and B (**8**) were isolated from the fungus *Microsphaeropsis* sp. The absolute configuration of palmarumycin M_1 (**1a**) was determined by single-crystal X-ray analysis of the bis(4-bromobenzoate) **1c** and the relationship between **1a**, **2** and **3** established by chemical transformation. The relative configuration of papyracillic acids A–C (**4**–**6**) was revised and their absolute configuration determined by comparison of TDDFT calculated and experimental solid-state CD spectra.



Keywords: Fungal secondary metabolites / Palmarumycins M / Papyracillic acids / Microsphaeropsins / *Microsphaeropsis* sp. / Solid-state CD / Exciton chirality

Mechanistic Studies

The $Sn(CF_3SO_3)_2$-catalyzed synthesis of 2,5-disubstituted tetrahydrofuran from a donor–acceptor cyclopropane cycloaddition reaction with benzaldehyde proceeds in a regio- and diastereoselective manner; the S_N2 mechanism was confirmed by density functional calculations.



Keywords: Density functional calculations / Tin / Donor–acceptor systems / Synthesis / Cycloaddition

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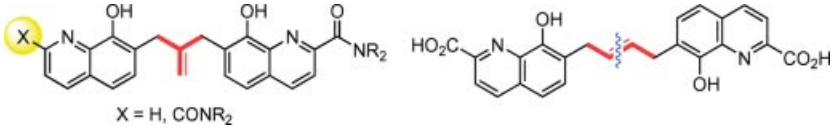
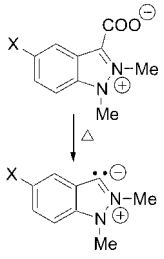
Ditopic Hydroxyquinolines



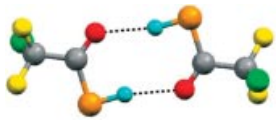
Homo- and heterotopic bischelating 8-hydroxyquinoline-based ligands with different spacer lengths can be prepared by utilizing a Claisen rearrangement as a central reaction step. The tandem Hiratani–Claisen reaction proved to be especially useful in this respect.

Nucleophilic Carbenes



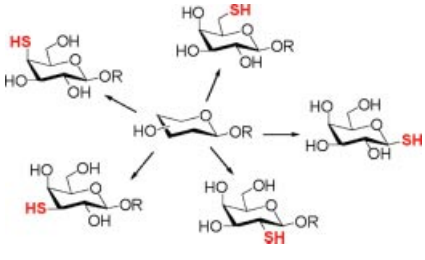
5-Fluoro-, chloro- bromo-, and iodo-substituted 1,2-dimethyl indazolium-3-carboxylates, members of the class of pseudo-cross-conjugated heterocyclic mesomeric betaines, undergo thermal decarboxylation to 5-halo-1,2-dimethyl-indazol-3-ylidenes. Physical analyses and trapping reactions with sulfur and 2,4-dichlorophenylisocyanate, respectively, are reported.

Halothioacetic Acid Chemistry



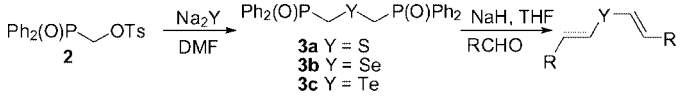
The novel thiocarboxylic acid $CF_2ClC(O)SH$ can be prepared from either $CF_2ClC(O)Cl$ or $[CF_2ClC(O)]_2O$. Its most stable form has a synperiplanar orientation of the C=O double bond with respect to the S–H single bond whereas the *gauche* orientation of the ClC–C=O moiety is preferred in the chlorodifluoroacetyl group. The crystal structure is formed from cyclic dimers bonded by weak hydrogen bonds.

Carbohydrate Synthesis



Systematic synthetic strategies to all positional thiol analogs of β-D-galactopyranose is presented.

Divinylic Chalcogenides



The preparation of bis[(diphenylphosphinoyl)methyl] sulfides, selenides, and tellurides is described. The title compounds are subjected to Horner–Wittig-type reactions with aldehydes and ketones to give symmetrical and unsymmetrical divinylic sulfides, selenides, and tellurides with preferential (*E*) stereochemistry.

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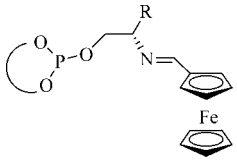
Asymmetric Catalysis

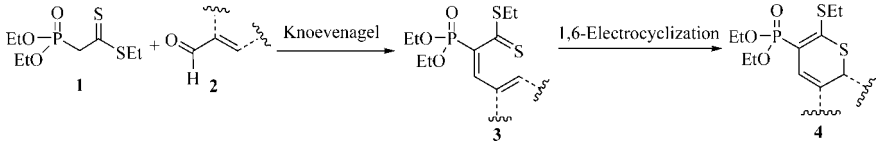


A family of ferrocenyliminophosphite ligands were successfully used in Rh-catalysed hydrogenations and Pd-catalysed allylic substitutions with enantiomeric excesses up to 97 %. Systematic variation of the ligand parameters indicates that enantioselectivities are determined by the nature of the phosphocentre and also by the substituent in the *C**HN fragment.

Keywords: Asymmetric catalysis / N,P ligands / Hydrogenation / Allylation

Thiopyrans by Electrocyclization

Keywords: Domino reaction / Heteroelectrocyclization / Knoevenagel reaction / Phosphonodithioester / Thiopyran



Knoevenagel-type condensations between phosphonodithioacetate **1** and α,β-unsaturated aldehydes **2** directly afford 5-phosphono-substituted 2*H*-thiopyrans **4**. Use of heteroaromatic aldehydes permit the consecutive heteroelectrocyclization of the triene intermediate **3**, provided that the aromatic character of the C5–C6 double bond is sufficiently decreased, which is the case for electron-deficient indole nuclei. This Knoevenagel/1,6-heteroelectrocyclization sequence represents a new domino process.

Isomerization Metathesis

Keywords: Isomerization / Ring-closing metathesis / Benzazepines / Dihydroisoquinolines

This study investigates the scope and limitations of an isomerization-RCM approach which was used for the synthesis of substituted 2,3-dihydro-1*H*-2-benzazepines and 1,2-dihydroisoquinolines.

If not otherwise indicated in the article, papers in issue 28 were published online on September 14, 2007

