

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Cover

Incorporating Acta Chemica Scandinavica



See D. M. Hodgson, M. A. H. Stent, B. Štefane and F. X. Wilson, page 1139 A representation of an achiral epoxide undergoing enantioselective alkylative double ring-opening, *via* a ternary (-)-sparteine-*i*PrLi-epoxide complex (image by K. Harrison).

xi



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Profile: Organic & Biomolecular Chemistry profiles Professor Thomas Carell



COMMUNICATIONS

Improving conversion and enantioselectivity in hydrogenation by combining different monodentate phosphoramidites; a new combinatorial approach in asymmetric catalysis

Diego Peña, Adriaan J. Minnaard, Jeroen A. F. Boogers, André H. M. de Vries, Johannes G. de Vries and Ben L. Feringa

The combination of monodentate ligands in the rhodiumcatalysed enantioselective hydrogenation enables a new approach when searching for the optimal activity and enantioselectivity in catalysis.





 $R^1 = R^2 = (CH_2)_4$



1101

110

COMMUNICATIONS

Dendritic metalloporphyrins with a *distal* H-bond donor as mimics of haemoglobin

Beatrice Felber, Carlos Calle, Paul Seiler, Arthur Schweiger and François Diederich

Dendritic iron(π) porphyrins featuring first- and second-generation aryl ether dendrons and different *distal* H-bonding ligands were prepared as model systems for haemoglobin.

Asymmetric hydrogenation of a 4,4-diaryl-3-butenoate; a novel approach to sertraline

Lee T. Boulton, Ian C. Lennon and Raymond McCague

The asymmetric hydrogenation of a selectively crystallised (E)-4,4-diaryl-3-butenoate with a rhodium-PhanePhos catalyst is described, providing an intermediate to the antidepressant sertraline.

A highly selective route to β -*C*-glycosides *via* nonselective samarium iodide induced coupling reactions

Sara Palmier, Boris Vauzeilles and Jean-Marie Beau

Reductive samariation of acetylated glycopyranosyl 2-pyridyl sulfones in the presence of aldehydes, followed by an oxidation–isomerization sequence, provides the corresponding *C*-glycosyl compounds with high β -selectivity.

Catalytic transfer hydrogenation of conjugated nitroalkenes using decaborane: synthesis of oximes

Seung Hwan Lee, Yong June Park and Cheol Min Yoon

 α , β -Unsaturated nitroalkenes are readily reduced to the corresponding aldoximes and ketoximes in good yields under mild reaction conditions.

ARTICLES

A2-Rhodopsin: a new fluorophore isolated from photoreceptor outer segments

Nathan Fishkin, Young-Pyo Jang, Yasuhiro Itagaki, Janet R. Sparrow and Koji Nakanishi

Elevated concentrations of all-*trans*-retinal in photoreceptor outer segments leads to the formation of A2-rhodopsin (A2-Rh), an unprecedented fluorescent rhodopsin adduct which consists of bisretinoids (A2) linked to each of three lysine residues in the protein and which exhibits an emission spectrum similar to A2E.

ii



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Org. Biomol. Chem., 2003,1 iii

Potassium trimethylsilanolate induced cleavage of 1,3-oxazolidin-2- and 5-ones, and application to the synthesis

Diane M. Coe, Rossana Perciaccante and Panaviotis A. Procopiou

A convenient and efficient method for the cleavage of 1,3-oxazolidin-5-ones and 1,3-oxazolidin-2-ones utilising potassium trimethylsilanolate in tetrahydrofuran.

Reaction of acetylenic esters and *N*-functionalized phosphazenes. 1,2- *versus* 1,4-addition of *N*-vinylic phosphazenes

Francisco Palacios, Concepción Alonso, Jaione Pagalday, Ana María Ochoa de Retana and Gloria Rubiales

Phosphazenes derived from aminophosphonates and *N*-vinylic phosphazenes are synthetic intermediates for the preparation of conjugated phosphazenes and phosphorus ylides heterodienes, and heterocycles.

Rapid cyanation of aryl iodides in water using microwave promotion

Riina K. Arvela, Nicholas E. Leadbeater, Hanna M. Torenius and Heather Tye

Using water in conjunction with microwave heating it is possible to prepare aryl nitriles from aryl iodides rapidly and in high yield.

α-Keto amides as precursors to heterocycles—generation and cycloaddition reactions of piperazin-5-one nitrones

Frances Heaney, Julie Fenlon, Patrick McArdle and Desmond Cunningham

A range of heterocyclic compounds *viz* ketopiperazine *N*-oxides, 1, isoxazolopyrrolidinones, 11, isoxazolidine- 13 and isoxazoline- 15 fused piperazinones and pyrrolopiperazinones 16 with potential for biological interest have been prepared from α -ketoamides 10.

Does the DABCO-catalysed reaction of 2-hydroxybenzaldehydes with methyl acrylate follow a Baylis-Hillman pathway?

Perry T. Kaye, Musiliyu A. Musa, Xolani W. Nocanda and Ross S. Robinson

In the formation of chromene and coumarin derivatives from DABCO-catalysed reactions of 2-hydroxybenzaldehydes with methyl acrylate it appears that: i) the Baylis–Hillman reaction *precedes* conjugate addition or acyl substitution; and ii) the pivotal intermediates are, in fact, highly activated dipolar adducts rather than the Baylis–Hillman products *per se*.



Q

TFDA, N

ARTICLES

Enantioselective alkylative double ring-opening of epoxides derived from cyclic allylic ethers: synthesis of enantioenriched unsaturated diols

David M. Hodgson, Matthew A. H. Stent, Bogdan Štefane and Francis X. Wilson

Enantioenriched unsaturated diols arise from epoxides of 2,5-dihydrofuran and oxabicyclo[n.2.1]alkenes (n = 2, 3) by using organolithiums and chiral ligands.

A novel approach of cycloaddition of difluorocarbene to α,β -unsaturated aldehydes and ketones: synthesis of *gem*-difluorocyclopropyl ketones and 2-fluorofurans

Wei Xu and Qing-Yun Chen

A series of *gem*-difluorocyclopropyl acetals and ketals are synthesized, which can be hydrolyzed to *gem*-difluorocyclopropyl ketones or 1-aryl-2-fluorofuran derivatives in the presence of oxalic acid.

The synthesis of trianglimines: on the scope and limitations of the [3 + 3] cyclocondensation reaction between (1R,2R)-diaminocyclohexane and aromatic dicarboxaldehydes

Nikolai Kuhnert, Giulia M. Rossignolo and Ana Lopez-Periago

The [3 + 3] cyclocondensation reaction with (1R,2R)-diaminocyclohexane and aromatic dicarboxaldehydes to give trianglimine macrocycles is discussed. The scope and limitations of the cyclocondensation reaction are studied and some comments on the properties of the novel macrocycles are made.

Reaction of hydroxyl radicals with *S*-nitrosothiols: determination of rate constants and end product analysis

Veleeparambil M. Manoj and Charuvila T. Aravindakumar

Evidence for the degradation of RSNOs induced by 'OH is presented. The high rate constants obtained for this reaction indicate the probable involvement of 'OH in the metabolism of *S*-nitrosoglutathione and *S*-nitrosocysteine.

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Oxalic acid

1170

1180

1157

$$RSNO + {}^{\bullet}OH \longrightarrow {}^{1}\!/_{2} RSSR + HNO_{2} (H^{+} + NO_{2}^{-})$$

Acidity of hydroxamic acids and amides

Stanislav Böhm and Otto Exner

Hydroxamic acids are relatively strong acids due to the acidity of the NH hydrogen. Is it caused entirely by the resonance in the anion? In the case of carboxylic acids, the importance of resonance was recently questioned.

$$CH_3C \xrightarrow{O}_{N=O}^{O} H \xrightarrow{CH_3C}_{N=O}^{O^{\ominus}} H$$

iv



ARTICLES

EPR and modelling studies of hydrogen-abstraction reactions relevant to polyolefin cross-linking and grafting chemistry

Susana Camara, Bruce C. Gilbert, Robert J. Meier, Martin van Duin and Adrian C. Whitwood

Calculated transition-state structures for H-abstraction from 2,4-dimethylpentane by *tert*-butoxyl.

X–N Charge density analysis of the hydrogen bonding motif in 1-(2-hydroxy-5-nitrophenyl)ethanone

David E. Hibbs, Jacob Overgaard and Ross O. Piltz

Fine details of intra- and intermolecular bonding features are revealed, in particular the extent of the π -delocalisation throughout the molecule.

Methyl radical also reacts by the frontside mechanism: An *ab initio* study of some homolytic substitution reactions of methyl radical at silicon, germanium and tin

Hiroshi Matsubara, Sonia M. Horvat and Carl H. Schiesser

Homolytic substitution of methyl radical at silicon, germanium and tin can proceed *via* both backside and frontside attack mechanisms.

Kinetics and mechanism of ring transformation of *S*-[1-(4-methoxyphenyl)pyrrolidin-2-on-3-yl]isothiuronium bromide to 2-methylimino-5-[2-(4-methoxyphenylamino)ethyl]-thiazolidin-4-one

Miloš Sedlák, Jiří Hanusek, Ludmila Hejtmánková and Pavla Kašparová

The transformation reaction is subject to general base, general acid, and hydroxide-ion catalyses.

1,3-Bis(diarylmethylidene)-2-methylidenecyclohexanes in cycloaddition and cyclodimerization reactions. The role of stereoelectronic factors

Elena I. Klimova, Marcos Martínez García, Tatiana Klimova, S. Hernandez Ortega and Leon V. Bakinovsky

Cycloaddition and cyclodimerization of the diaryltrienes are studied. In the presence of CF₃COOH, a central, 'three-petal' fragment of six-membered rings is formed.



ARTICLES

The synthesis and studies towards the self-replication of bis(capped porphyrins)

Pall Thordarson, Annie Marquis and Maxwell J. Crossley

The *syn-* and *anti-*bis(capped porphyrins) can catalyse their own formation but not by a self-replication pathway.

Synthetic multifunctional pores: deletion and inversion of anion/cation selectivity using pM and pH

Naomi Sakai, Nathalie Sordé, Gopal Das, Philippe Perrottet, David Gerard and Stefan Matile

Internal counterion immobilization is used to construct supramolecular pores with attractive properties such as superb stability and multifunctionality.

Halo-Derivatised Calix[4]tubes

Susan E. Matthews, Vitor Felix, Michael G. B. Drew and Paul D. Beer

Novel halo-derivatised calix[4]tubes exhibit exceptional selectivity for potassium as evidenced by NMR, ESMS and molecular modelling studies.

Carboxylic acid clathrate hosts of Diels–Alder adducts of phencyclone and 2-alkenoic acids. Role of bidentate $C-H \cdots O$ hydrogen bonds between the phenanthrene and carbonyl groups in host–host networks

Yasuyuki Yoshitake, Junichi Misaka, Masaki Abe, Masatoshi Yamasaki, Masashi Eto and Kazunobu Harano

The carboxylic acid hosts of the *endo* DA adducts of phencyclone and 2-alkenoic acids showed high inclusion ability for different types of guests.