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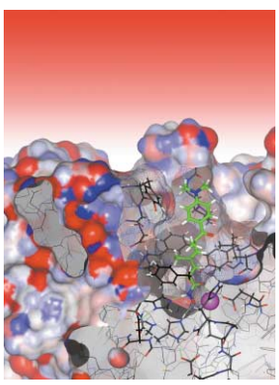
Organic & Biomolecular Chemistry

FORMERLY PERKIN TRANSACTIONS 1 AND 2

Incorporating Acta Chemica Scandinavica



Cover
See K. Vanommeslaeghe, C. Van Alsenoy, F. De Proft, J. C. Martins, D. Tourwé and P. Geerlings, page 2951.
The calculated structure of the potent HDAC inhibitor TSA, binding to an HDAC analogue. A solvent accessible surface around the protein is displayed, partially cut away to reveal the underlying active site, in which the catalytic zinc ion and some relevant polar interactions are highlighted.

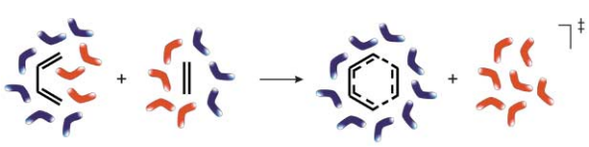
contents

PERSPECTIVE

Hydrophobic interactions and chemical reactivity

Sijbren Otto and Jan B. F. N. Engberts

The influence of hydrophobic interactions on rates of chemical reactions can be a useful tool in organic synthesis as well as for the study of these hydrophobic interactions.

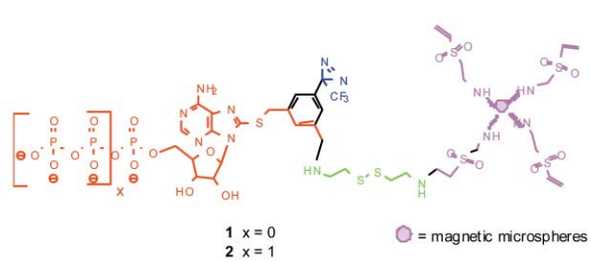


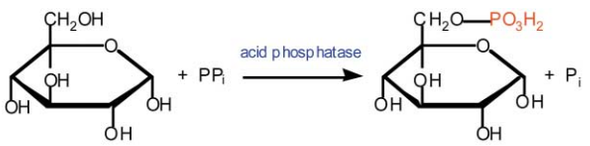
ARTICLES

Photoaffinity labeling on magnetic microspheres (PALMm) methodology for topographic mapping: preparation of PALMm reagents and demonstration of biochemical relevance

Efrat Halbfinger, Karine Gorochesky, Sébastien A. Lévesque, Adrien R. Beaudoin, Larisa Sheihet, Shlomo Margel and Bilha Fischer

PALMm reagents bound to magnetic-microspheres were designed and evaluated for the topographic mapping of ATP-binding proteins.

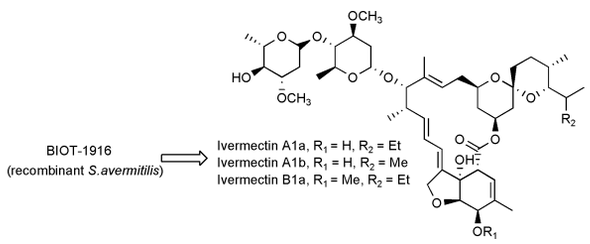




Phosphorylation and dephosphorylation of polyhydroxy compounds by class A bacterial acid phosphatases

Naoko Tanaka, Zulfiqar Hasan, Aloysius F. Hartog, Teunie van Herk and Ron Wever

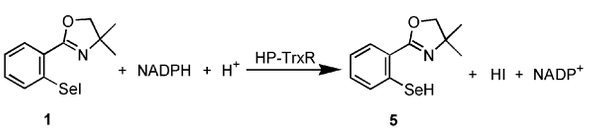
A novel enzymatic method to phosphorylate glucose regioselectively to glucose 6-phosphate by bacterial acid phosphatase.



Direct production of ivermectin-like drugs after domain exchange in the avermectin polyketide synthase of *Streptomyces avermitilis* ATCC31272

S. Gaisser, L. Kellenberger, A. L. Kaja, A. J. Weston, R. E. Lill, G. Wirtz, S. G. Kendrew, L. Low, R. M. Sheridan, B. Wilkinson, I. S. Galloway, K. Stutzman-Engwall, H. A. I. McArthur, J. Staunton and P. F. Leadlay

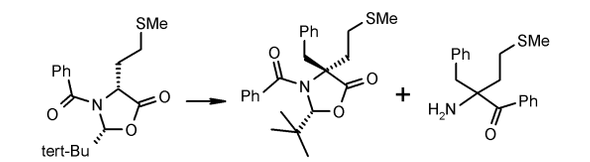
Production of 22,23-dihydroavermectins B1a **9** and A1a **11** by direct fermentation of a recombinant strain of *Streptomyces avermitilis* ATCC31272 containing an appropriately-engineered polyketide synthase.



Selenenyl iodide: a new substrate for mammalian thioredoxin reductase

Govindasamy Mugesh, Lars-Oliver Klotz, Wolf-Walther du Mont, Katja Becker and Helmut Sies

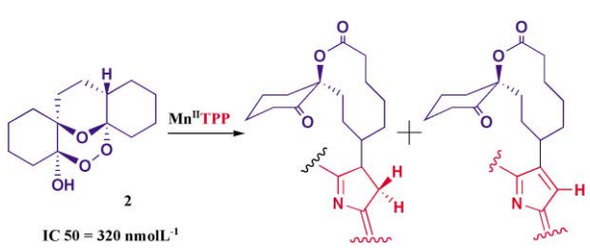
Areneselenenyl iodide stabilised by internal chelation has been synthesized and evaluated as a substrate of thioredoxin reductase (TrxR).



Synthesis of (*R*)-α-benzylmethionine: a novel rearrangement during alkylation of the Seebach (*R*)-methionine oxazolidinone

Panayiotis A. Procopiou, Mahmood Ahmed, Séverine Jeulin and Rossana Perciaccante

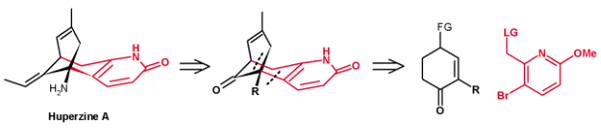
A novel amino ketone by-product was observed during alkylation of the oxazolidinone with BnBr.

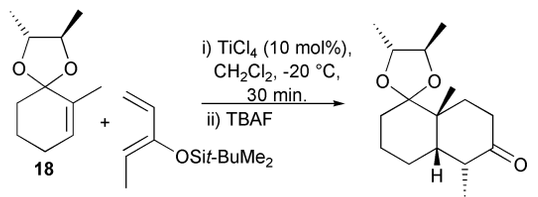


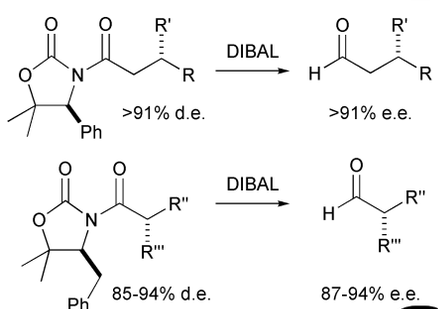
Alkylation of manganese(II) tetraphenylporphyrin by a synthetic antimalarial trioxane

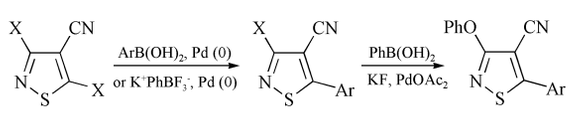
Jean-François Berrien, Olivier Provot, Joëlle Mayrargue, Michel Coquillay, Liliane Cicéron, Frédérick Gay, Martin Danis, Anne Robert and Bernard Meunier

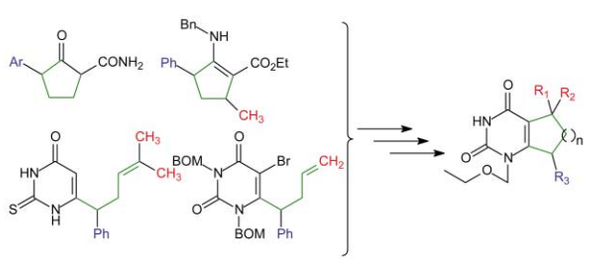
The alkylation of manganese(II) tetraphenylporphyrin ($Mn^{II}TPP$) by trioxane **2** is presented.

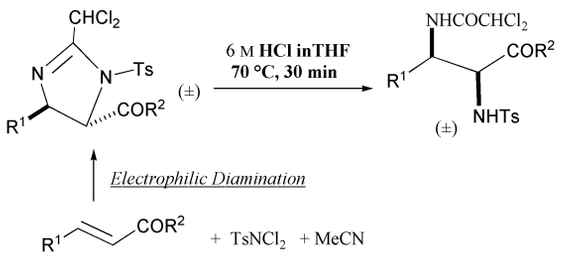








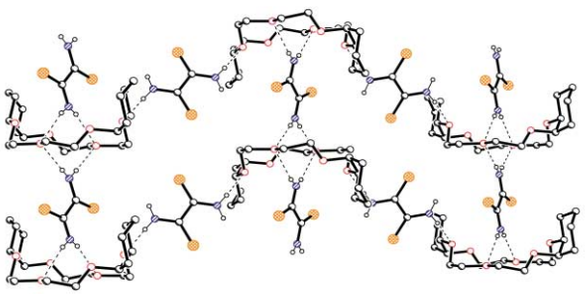




Novel imidazolination reaction of alkenes provides an easy access to new α,β-differentiated 1,2-vicinal diamines

Wei Pei, Cody Timmons, Xin Xu, Han-Xun Wei and Guigen Li

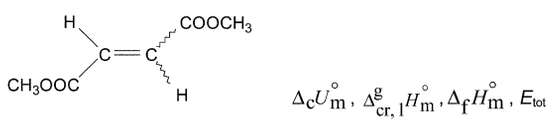
α,β-Diamino esters which are α and β-amino acid mimics were synthesized by hydrolyzing new imidazolines.



From 1D strands to extended molecular assemblies in the binary compounds of dithiooxamide and dithiobiurea with crown ethers

Yurii A. Simonov, Marina S. Fonari, Michael J. Zaworotko, Heba Abourahma, Janusz Lipkowski, Edward V. Ganin and Arkadii A. Yavolovskii

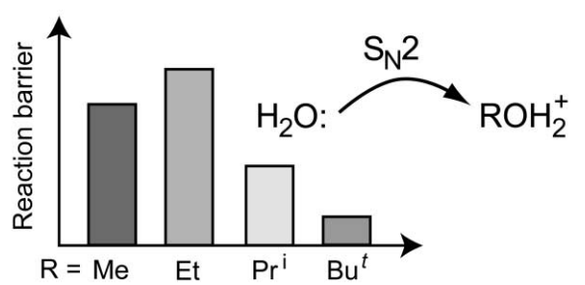
Binary compounds of dithiooxamide/dithiobiurea with crown ethers exhibit a diversity of structural types in the crystal.



Thermochemistry of (*E*)- and (*Z*)-disubstituted alkene species: a combined experimental and theoretical investigation of isomeric dimethyl fumarate and dimethyl maleate

M. Agostinha R. Matos, Margarida S. Miranda, Victor M. F. Morais and Joel F. Liebman

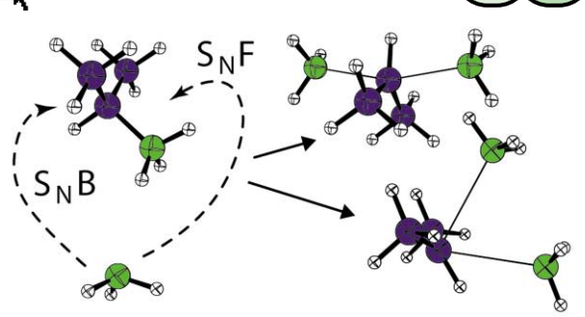
Thermochemistry of isomeric dimethyl fumarate and dimethyl maleate: a combined experimental and theoretical investigation of enthalpies and energies.



Nucleophilic identity substitution reactions. The reaction between water and protonated alcohols

Jon K. Laerdahl and Einar Uggerud

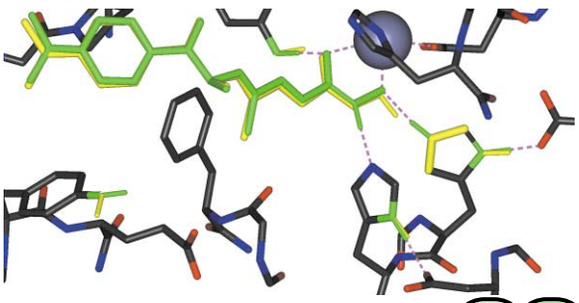
Competing front- and rear-side nucleophilic substitution and inverse relationship between S_N2 reaction barriers and "steric effects" investigated for the $H_2O + ROH_2^+$ (R = Me, Et, Pr^i, Bu^t) reaction.



Nucleophilic identity substitution reactions. The reaction between ammonia and protonated amines

Jon K. Laerdahl, Lihn Bache-Andreassen and Einar Uggerud

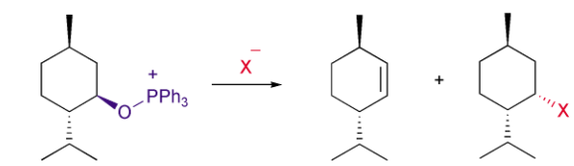
Nucleophilic substitution and elimination reactions have been investigated for the $NH_3 + RNH_3^+$ (R = Me, Et, Pr^i, Bu^t) systems. Reaction barrier trends have been compared with similar systems and analyzed in terms of bond strengths and charge development on the leaving group and reaction centre.



Ab initio study of the binding of Trichostatin A (TSA) in the active site of Histone Deacetylase Like Protein (HDLP)

Kenno Vanommeslaeghe, Christian Van Alsenoy, Frank De Proft, José C. Martins, Dirk Tourwé and Paul Geerlings

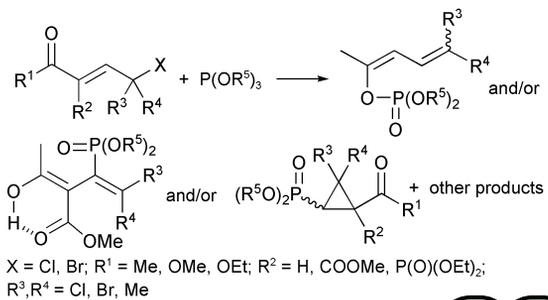
Theoretical study of the binding of TSA and water to HDLP, providing insight into the mechanism of action.



The Hendrickson reagent and the Mitsunobu reaction: a mechanistic study

Kathryn E. Elson, Ian D. Jenkins and Wendy A. Loughlin

The same alkoxytriphenylphosphonium ion intermediate is generated from menthol using either the Hendrickson reagent or the Mitsunobu reaction, but one reaction leads mainly to elimination, the other to substitution. Why?

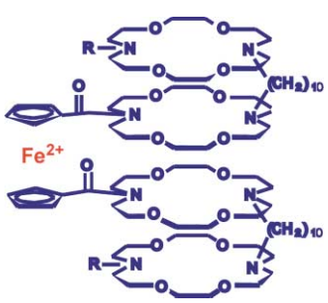


X = Cl, Br; R^1 = Me, OMe, OEt; R^2 = H, COOMe, P(O)(OEt)$_2$; R^3,R^4 = Cl, Br, Me

Mechanistic and synthetic aspects of the reaction of γ-halogeno-α,β-unsaturated ketones and esters with simple trialkyl phosphites

Wiesław Waszkuć and Tomasz Janecki

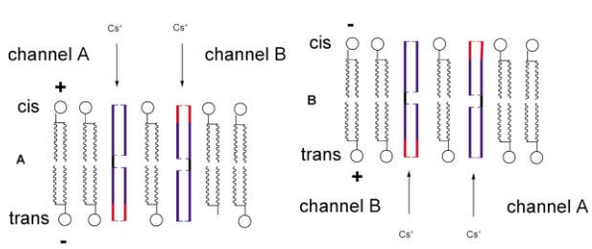
The main products of the title reaction were characterized and a plausible mechanism for their formation was proposed.



Cation transport by a redox-active synthetic ion channel

Adam C. Hall, Cristina Suarez, Anindita Hom-Choudhury, Aida N. A. Manu, C. Dennis Hall, Gregory J. Kirkovits and Ion Ghiriviga

Synthesis, cation binding and sodium flux properties of a novel synthetic ion channel containing a redox-active centre.



Synthesis and functional studies of THF–gramicidin hybrid ion channels

Andrea Vescovi, Andrea Knoll and Ulrich Koert

Replacement of positions 10 and 11 of gramicidin A by a D-THF amino acid gave rise to new and interesting channel properties. Most remarkable is the asymmetric compound **8**, which inserts selectively into a DPhPC membrane and displays voltage-directed gating dynamics.

CONFERENCE DIARY

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Dates, venues and contact details of forthcoming events.

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