

## JOURNAL OF THE CHEMICAL SOCIETY

**Perkin Transactions 2**

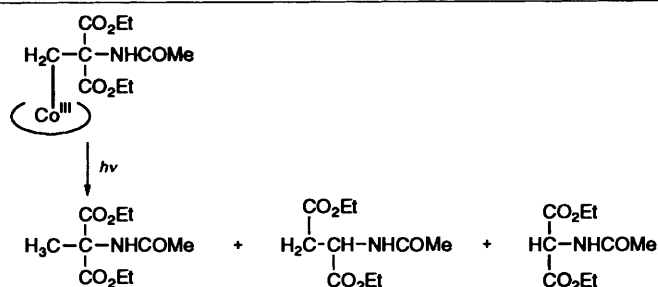
## Physical Organic Chemistry

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## Perkin Communications

- 189 **Carbon-skeleton rearrangement of an amino acid derivative as mediated by hydrophobic vitamin B<sub>12</sub> covalently bound to a lipid species in a bilayer membrane**

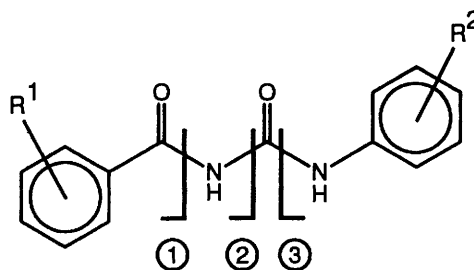
Yukito Murakami, Yoshio Hisaeda,  
Akihiro Ogawa and Teruhisa Ohno



## Articles

- 193 **Computer-assisted prediction of the degradation of chemicals: hydrolysis of amides and benzoylphenylureas**

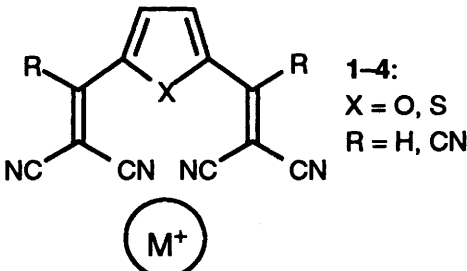
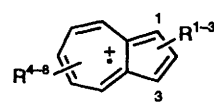
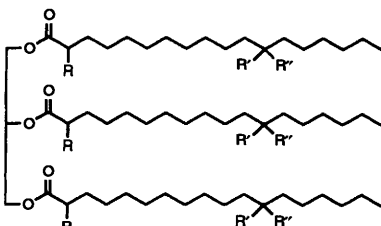
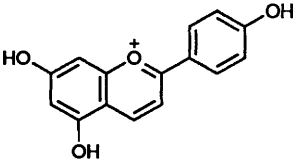
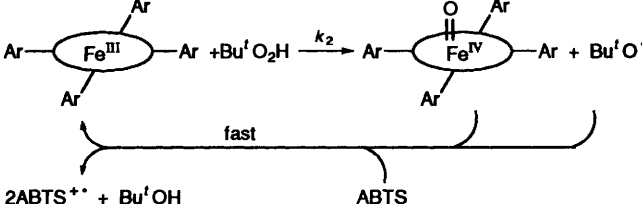
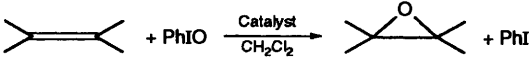
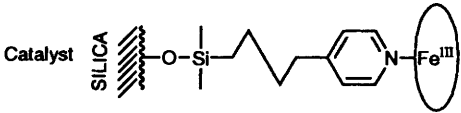
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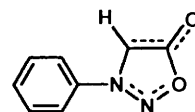


- 205 **Protonation and acid catalysed hydrolysis of nitrosoaryl ethers**

Roy B. Moodie and Brian O'Sullivan

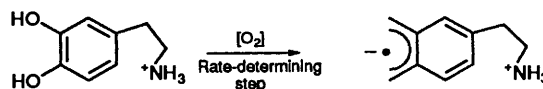


<p>209 <b>Factors determining ion-pair formation. Studies of the radical anions of 2,5-bis(tricyanovinyl)-furan and 2,5-bis(tricyanovinyl)thiophene</b></p> <p>Markus Scholz, Georg Gescheidt, Ulrich Schöberl and Jörg Daub</p>	 <p>1-4: X = O, S R = H, CN</p> <p>Radical anions of 1-4 form ion-pairs with alkali metals depending upon the distance between facing N-atoms and cation size</p>
<p>215 <b>Radical cations of alkylazulenes: an EPR and ENDOR study</b></p> <p>Fabian Gerson, Markus Scholz, Hans-Jürgen Hansen and Peter Uebelhart</p>	 <p>Radical cations of azulenes bearing alkyl groups in the reactive 1,3-positions were persistent enough in a stationary system to be characterized by their hyperfine data, whereas those lacking one or both such substituents rapidly yielded the radical cations of corresponding 1,1'-biazulenylys</p>
<p>221 <b>Synthesis and characterisation of selectively fluorinated stearic acids (octadecanoic acids) and their tristearins: the effect of introducing one and two fluorine atoms into a hydrocarbon chain</b></p> <p>Lakkaraju Dasaradhi, David O'Hagan, Michael C. Petty and Christopher Pearson</p>	 <p>The physical properties of the CHF and CF<sub>2</sub> substituted tristearins 2-4 are reported</p> <p>1 R = R' = R'' = H    2 R = F, R' = R'' = H 3 R = R' = H, R'' = F    4 R = H, R' = R'' = F</p>
<p>227 <b>Quantitative measurement of proton dissociation and tautomeric constants of apigeninidin</b></p> <p>Luca Costantino, Giulio Rastelli, Maria C. Rossi and Albano Albasini</p>	 <p>A quantitative description of proton dissociations and tautomeric equilibria of apigeninidin in solution is reported</p>
<p>235 <b>A kinetic study of the reaction of <i>tert</i>-butyl hydroperoxide with iron(III) 5,10,15,20-tetra(4-sulfonatophenyl)porphyrin and related compounds in aqueous solution</b></p> <p>Nicola Colclough and John R. Lindsay Smith</p>	 <p>2,2'-Azinobis(3-ethyl-2,3-dihydrobenzothiazole-6-sulfonate) (ABTS) has been used as an oxidant trap to study the pH dependence of <math>k_2</math></p>
<p>243 <b>Alkene epoxidation by iodosylbenzene catalysed by iron(III) 5,10,15,20-tetra(2,6-dichlorophenyl)porphyrin coordinated to pyridine-modified silica</b></p> <p>Claire Gilmartin and John R. Lindsay Smith</p>	 

253 **Theoretical studies on the structure and electronic properties of 3-(4-tolyl)sydnone**

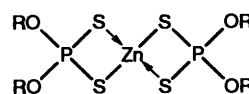
Calculated structure and dipole moment

John O. Morley

259 **Spontaneous autoxidation of dopamine**

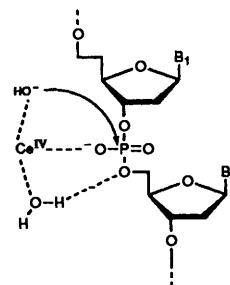
The reaction between dopamine, 2-(3,4-dihydroxyphenyl)-ethylamine, and dioxygen in neutral to slightly alkaline aqueous solution has been investigated; a simple rate law is found and a mechanism proposed, and the role of metal ions on the course of this reaction is discussed

Erwin Herlinger, Reginald F. Jameson and Wolfgang Linert

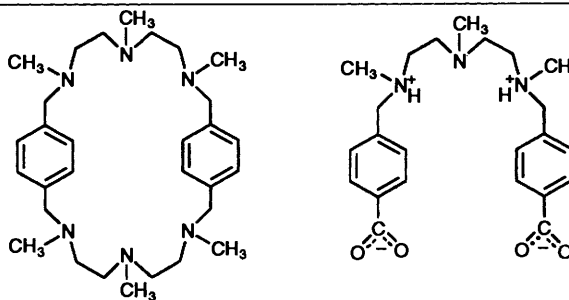
265 **Phosphorus-31 NMR investigation of the heterogeneous hydrolytic decomposition of zinc(II) bis(*O,O*-dialkyl dithiophosphate) lubricant additives**

Relative rates of heterogeneous-phase hydrolytic breakdown decrease significantly as size of the alkyl group R increases; the rate-limiting step of the process is attributed to diffusion across the solvent-water interface

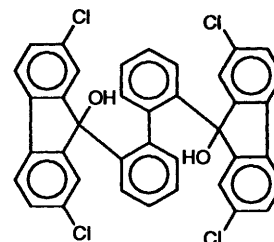
Alan J. Burn, Ian Gosney, Chris P. Warrens and John P. Wastle

269 **Efficient and oxygen-independent hydrolysis of single-stranded DNA by cerium(IV) ion**

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275 **Basicity properties of a novel azaparacyclophane receptor and its acyclic precursor: a thermodynamic and structural approach**

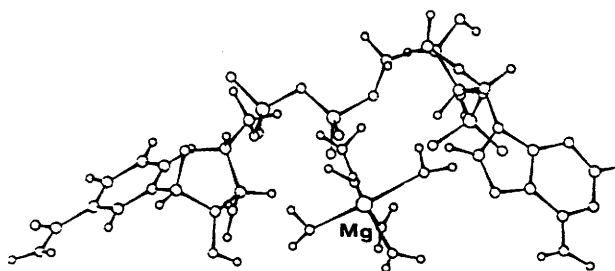
Carla Bazzicalupi, Andrea Bencini, Antonio Bianchi, Vieri Fusi, Claudia Giorgi, Piero Paoletti, Annalisa Stefani and Barbara Valtancoli

281 **Complexation with diol host compounds. Part 20. Kinetics of desolvation of inclusion compounds of 2,2'-bis(2,7-dichloro-9-hydroxy-9-fluorenyl)biphenyl with 1,4-dioxane and 1,3-dioxolane**

Mino R. Caira, Anita Coetzee, Luigi R. Nassimbeni, Edwin Weber and Andreas Wierig

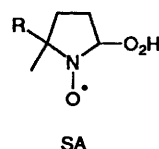
285 Interaction between metal ions and NAD(P) coenzymes.  $^1\text{H}$ ,  $^{31}\text{P}$ ,  $^{13}\text{C}$  and  $^{59}\text{Co}$  NMR spectroscopy and conformational analysis

Stefania Mazzini, Rosanna Mondelli, Enzo Ragg and Leonardo Scaglioni



295 Decay of the hydroperoxyl spin adduct of 5-diethoxyphosphoryl-5-methyl-1-pyrroline *N*-oxide: an EPR kinetic study

Béatrice Tuccio, Robert Lauricella, Claudine Fréjaville, Jean-Claude Bouteiller and Paul Tordo



$\text{R} = \text{CH}_3, \text{P}(\text{O})(\text{OEt})_2$

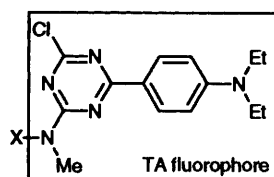
$$-d[\text{SA}]/dt = k_a[\text{SA}] + k_b[\text{SA}]^2$$

SA

SA decay was monitored by EPR spectroscopy

299 Triazinylaniline (TA) derivatives as fluorescence probes. Part 2. Steady-state and time-resolved fluorescence anisotropy studies of TA probes in alkanols and in small unilamellar vesicles of phospholipids

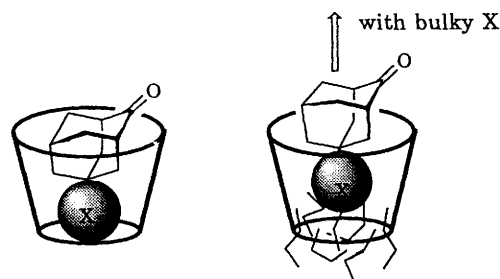
David J. Cowley and Richard S. J. Todd



Rotation in DMPC and DPPC bilayers as a function of anchor group X = butyl, octadecyl and  $-\text{CH}_2[\text{CHOH}]_4\text{CH}_2\text{OH}$

307 Photocycloaddition of fumaronitrile to adamantan-2-ones and modification of face selectivity by inclusion in  $\beta$ -cyclodextrin and its derivatives

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315 Organophosphorus compounds. Part 93. Aromaticity of thia- and selenaphospholes: a photoelectron spectroscopic and quantum chemical study

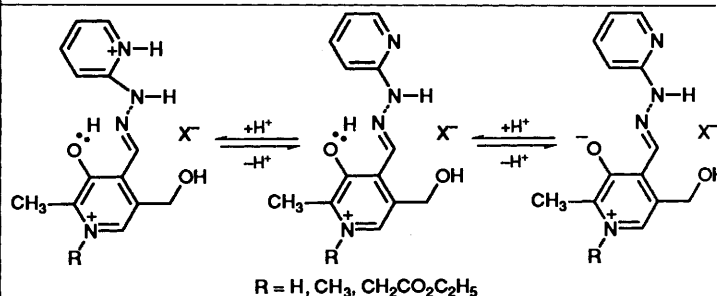
László Nyulászi, Péter Várnai, Steffen Krill and Manfred Regitz

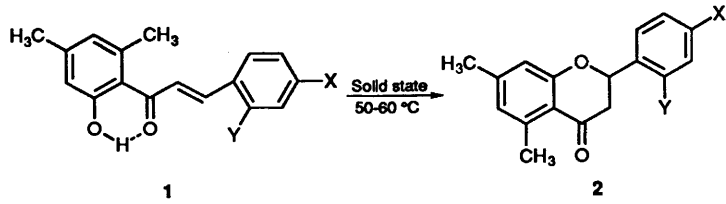
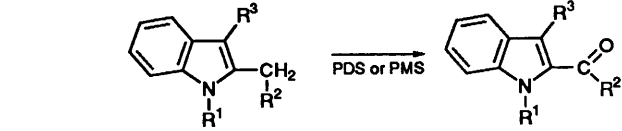
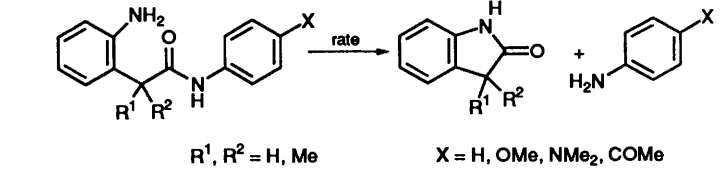
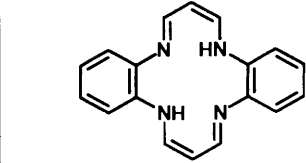
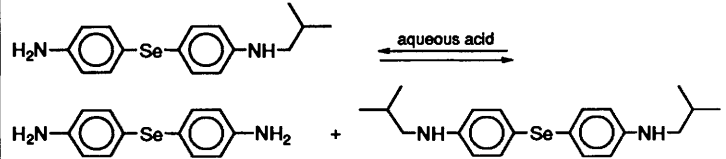
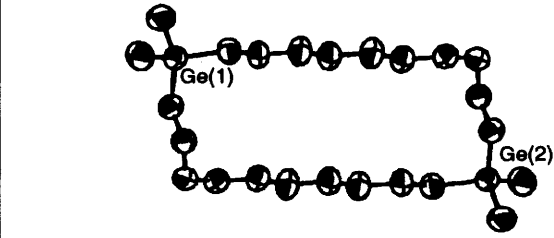


The aromatic character of thia- and selenaphospholes as well as thia- and selenadiphospholes has been investigated by photoelectron spectroscopy and quantum chemical calculations

319 Iron chelators of the pyridoxal 2-pyridyl hydrazone class. Part 4.  $\text{p}K_a$  values of the chelators and their relevance to biological properties

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<p>325 <b>Intramolecular Michael-type addition in the solid state</b></p> <p>B. Satish Goud, Kaliyamoorthy Panneerselvam, David E. Zacharias and Gautam R. Desiraju</p>	
<p>331 <b>Kinetics and mechanisms of the oxidation reactions of some 2,3-dialkylindole derivatives by peroxydisulfate and peroxymonosulfate anions</b></p> <p>Carmen Carmona, Manuel Balón, María A. Muñoz, Pilar Guardado and José Hidalgo</p>	
<p>337 <b>Kinetics and mechanism of the cyclization of substituted <i>N</i>-phenyl-2-methyl-2-(2-amino-phenyl)propanamides and analogues</b></p> <p>Bridget M. Sykes, Graham J. Atwell, William A. Denny, Duncan J. McLennan and Charmian J. O'Connor</p>	 <p style="text-align: center;"><math>R^1, R^2 = H, Me</math>                      <math>X = H, OMe, NMe_2, COMe</math></p>
<p>343 <b>A crystal modification of dibenzo[<i>b,i</i>]-[1,4,8,11]tetraaza[14]annulene: X-ray molecular structure and proton tautomerism of the highly <math>\pi</math>-conjugated form</b></p> <p>Nagao Azuma, Hiroyuki Tani, Takehiro Ozawa, Hiroko Niida, Kunihiro Tajima and Kazunori Sakata</p>	 <p>The imine-enamine tautomerization was suggested by an X-ray crystallographic study and observed by NMR measurement in [<sup>2</sup>H<sub>8</sub>]toluene even at -90 °C</p>
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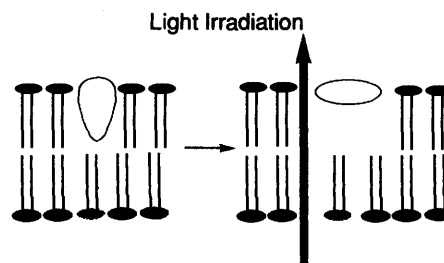
359 Destabilization of the heme region in mutant cytochrome c by replacement of Phe-82 with 3-(pyren-1-yl)-L-alanine

Takehiko Ueda, Shunsaku Kimura and Yukio Imanishi



365 Photoresponsive melittin having a spiropyran residue in the hydrophobic region of the sequence

Takehiko Ueda, Koichi Nagamine, Shunsaku Kimura and Yukio Imanishi



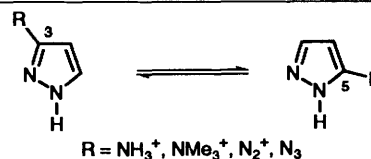
369 Hydrogen bonding. Part 29. Characterization of 14 sorbent coatings for chemical microsensors using a new solvation equation

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379 Theoretical calculations on pyrazole derivatives. Part 2. Effect of cationic C-substituents ( $\text{NH}_3^+$  and  $\text{N}_2^+$ ) on the basicity and tautomerism of pyrazoles

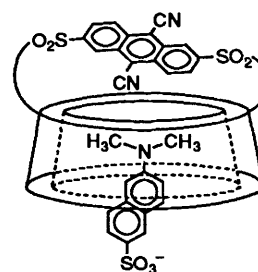
Abdellatif El Hammadi, Mohamed El Mouhtadi, Rafael Notario, Andreas Werner and José Elguero



AM1 and, in some cases, 6-31G calculated proton affinities show that positively charged substituents shift the above equilibrium towards the 3-substituted tautomer; in the case of the diazonium group this prediction has been verified experimentally

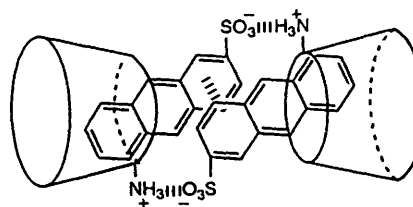
385 Static and dynamic fluorescence quenching of a dicyanoanthracene-capped  $\beta$ -cyclodextrin

Michael F. Acquavella, Mary E. Evans, Steven W. Farragher, Cédrine J. Névoret and Christopher J. Abelt

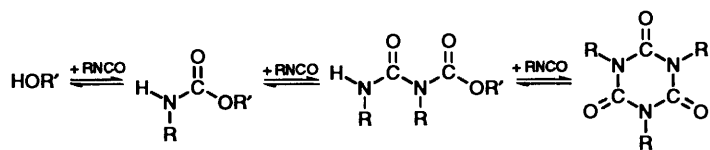


389 Complexation and photodimerization of anthracene-2-sulfonate in the presence of per-6-aminocyclodextrins

Seizo Tamagaki, Kazuyuki Fukuda, Hideyuki Maeda, Norimasa Mimura and Waichiro Tagaki

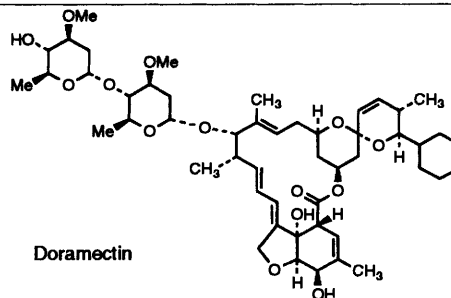


395 **Kinetics and catalysis of consecutive isocyanate reactions. Formation of carbamates, allophanates and isocyanurates**



Klaus Schwetlick and Rainer Noack

403 **Structure of doramectin**



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NOTE: An asterisk in the heading of each paper indicates the author who is to receive any correspondence.



## Forthcoming Articles in *Perkin Transactions 2*

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Substituent chemical shifts (SCSs) in NMR spectroscopy. Part 5. Mono- and di-fluoro SCSs in rigid molecules  
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<sup>17</sup>O and <sup>13</sup>C NMR spectra of stable simple enols **J. Frey, I. Eventova, Z. Rappoport, T. Müller, Y. Takai and M. Sawada**

Mechanism of rearrangement reactions of ketenimine–4-acylfuran-2,3-dione cycloadducts—a semiempirical molecular orbital study  
**W. M. F. Fabian and G. Kollenz**

Thermolysis of highly congested tri-*tert*-alkylmethanes. Rearrangement of a 3-noradamantylmethyl radical **J. S. Lomas**

Carbanion reactivity; kinetics of the reactions of benzyl cyanide anions with aromatic nitro-compounds  
**J. H. Atherton, M. R. Crampton, G. L. Duffield and J. A. Stevens**

Aliphatic radicals from ethers *via* photoinduced electron transfer: selective formation and chemistry  
**E. Fasani, M. Mella and A. Albini**

Channel-type molecular structures. Part 4. Transmembrane transport of alkali-metal ions by 'bouquet' molecules  
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