

JOURNAL OF THE CHEMICAL SOCIETY

Perkin Transactions 2

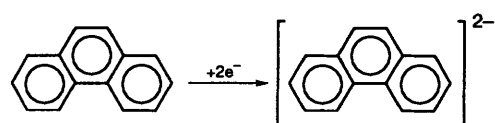
Physical Organic Chemistry

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Perkin Communications

1115 **Phenanthrene dianion is not planar**

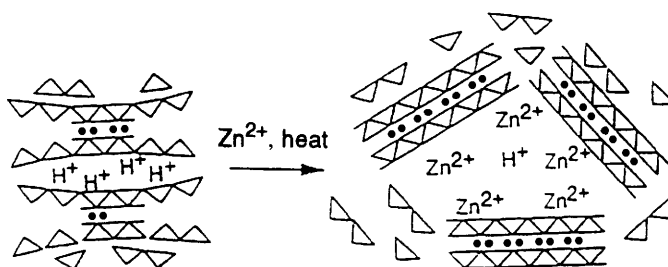
Aleksander Ioffe, Ari Ayalon and Mordecai Rabinovitz



Articles

Keynote Article1117 **Environmentally friendly chemistry using supported reagent catalysts: structure-property relationships for clayzic**

James H. Clark, and in part Stephen R. Cullen, Simon J. Barlow and Tony W. Bastock

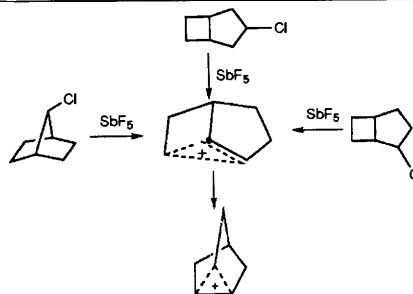
1131 **Transnitrosation between nitrosothiols and thiols**

D. Jonathan Barnett, John McAninly and D. Lyn H. Williams

Reaction occurs directly without prior formation of NO^+ or NO

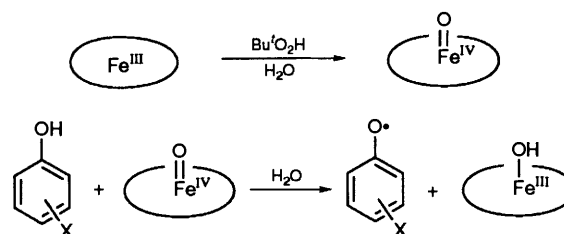
1135 **Rearrangement of bicyclo[3.2.0]heptyl precursors to the 7-norbornyl cation in the cryogenic SbF_5 matrix**

Milan Mesić, Dionis E. Sunko and Hrvoj Vančik



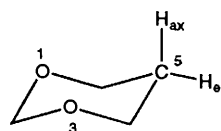
1139 **A mechanistic study of the oxidation of phenols in aqueous solution by oxoiron(IV) tetra(*N*-methylpyridyl)porphyrins. A model for horseradish peroxidase compound II?**

Nicola Colclough and John R. Lindsay Smith



1151 **NMR parameters for 1,3-dioxanes: evidence for a homoanomeric interaction**

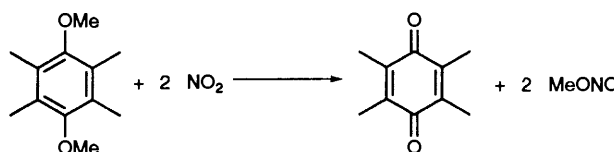
Jiaqiang Cai, Alwyn G. Davies and Carl H. Schiesser



The effect at the 5-position of the two β -oxygen atom is to reduce $^1J_{\text{C-H(eq)}}$ (ca. 125 Hz) relative to $^1J_{\text{C-H(ax)}}$ (ca. 132 Hz)

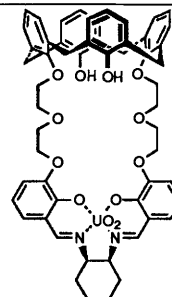
1157 **Oxidative dealkylation of hydroquinone ethers with nitrogen dioxide in the convenient preparation of quinones**

Rajendra Rathore, Eric Bosch and Jay K. Kochi



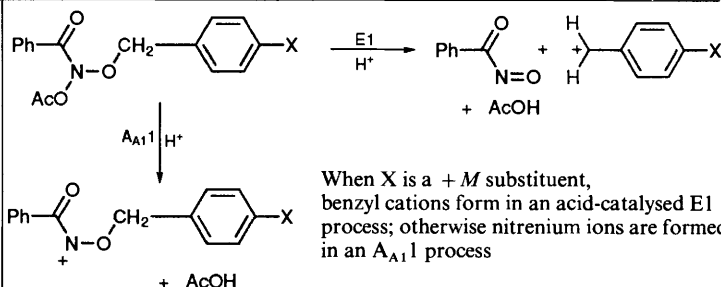
1167 **Calix salophen crown ethers as receptors for neutral molecules**

Arjen M. Reichwein, Willem Verboom, Sybolt Harkema, Anthony L. Spek and David N. Reinhoudt



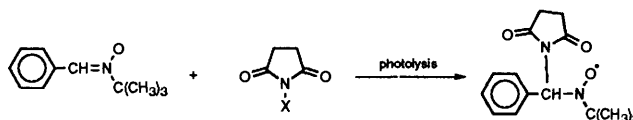
1173 **Reactive intermediates from the solvolysis of mutagenic *O*-alkyl *N*-acetoxybenzohydroxamates**

Antonio M. Bonin, Stephen A. Glover and Gerard P. Hammond



1181 **Inverted spin trapping. Part IV. Application to the formation of imidyl spin adducts from *N*-haloimides**

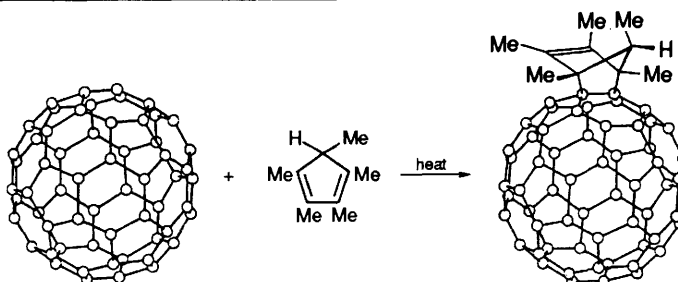
Lennart Ebersson, Johan Lind and Gabor Merenyi



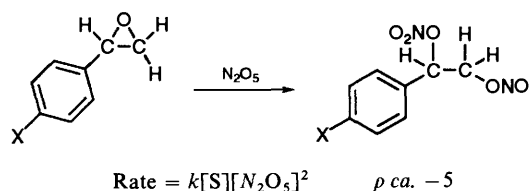
Imidyl spin adducts, formed by photolysis of *N*-haloimide-spin trap mixtures, are, in most cases, generated by photooxidation of the spin trap to its radical cation, followed by reaction of the latter with imide ion (inverse spin trapping)

1189 **Pentamethylcyclopentadiene adducts of [60]- and [70]-fullerene**

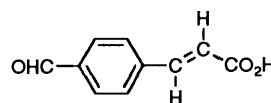
Mohamed F. Meidine, Anthony G. Avent, Adam D. Darwish, Harold W. Kroto, Osamu Ohashi, Roger Taylor and David R. M. Walton

1195 **Kinetics and mechanism of reaction of aryl oxiranes with dinitrogen pentoxide in dichloromethane**

Jonathan Dormer and Roy B. Moodie

1201 **The rôle of powder diffraction in establishing structure-property relationships for crystalline solids: a new structural assignment of the photoreactive and photostable phases of *p*-formyl-*trans*-cinnamic acid**

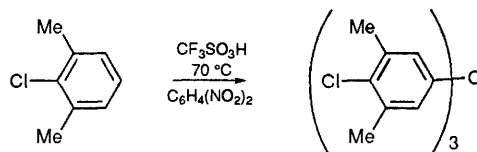
Kenneth D. M. Harris and Iain L. J. Patterson



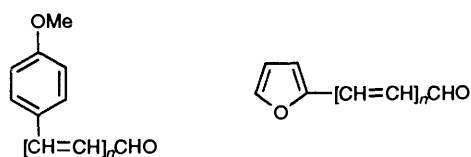
p-Formyl-*trans*-cinnamic acid can exist in two different crystalline phases—a photoreactive (β) phase and a photostable (γ) phase; powder X-ray diffraction has been applied to probe the relationship between crystal structure and photoreactivity in this system

1205 **Oxidation reduction reactions involving nitro groups in trifluoromethanesulfonic acid. Part 2. The reactions of chloromethylbenzenes with aromatic nitro compounds**

Rupert P. Austin and John H. Ridd

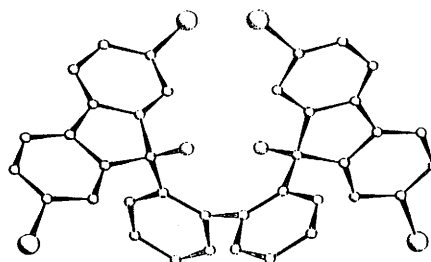
1211 **Nonlinear optical properties of organic molecules. Part 15. Calculation of the structure and hyperpolarisabilities of arylalkenes containing weak donors and acceptors**

John O. Morley



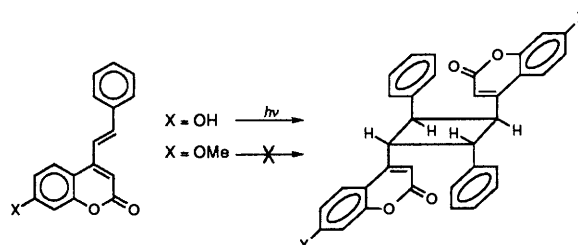
- 1215 **Crystalline inclusion compounds of substituted 2,2'-bis(9-hydroxyfluoren-9-yl)biphenyls: synthesis, X-ray crystal structures and thermal analysis study of inclusion compounds with butyronitrile, cyclohexanone, cyclopentanol and dimethylformamide**

Susan A. Bourne, Luigi R. Nassimbeni, Margaret L. Niven, Edwin Weber and Andreas Wierig



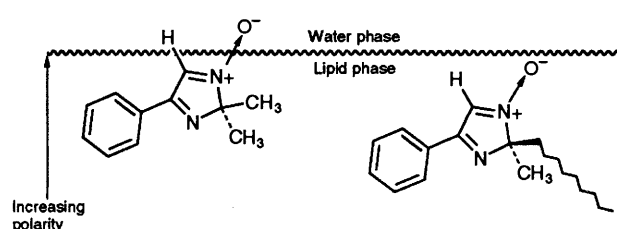
- 1223 **Studies in crystal engineering: structure-reactivity correlations of substituted styrylcoumarins and related systems**

J. Narasimha Moorthy, S. D. Samant and K. Venkatesan



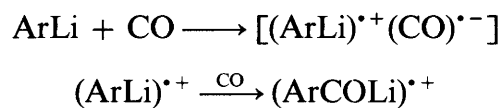
- 1229 **Determining the location of hydrophobic spin traps within liposomes**

Gila Strul, Hugo E. Gottlieb, Aryeh A. Frimer and Lev Weiner



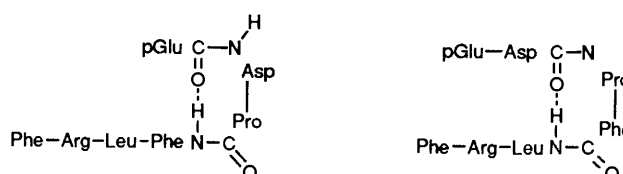
- 1233 **Kinetic study of the reaction of naphthyllithium with carbon monoxide in hexane-tetrahydrofuran solution**

N. Sbarbati Nudelman and Fabio Doctorovich



- 1239 **Conformational studies on analogues of the invertebrate peptide pyroGlu-Asp-Pro-Phe-Leu-Arg-Phe-NH₂ using ¹H NMR**

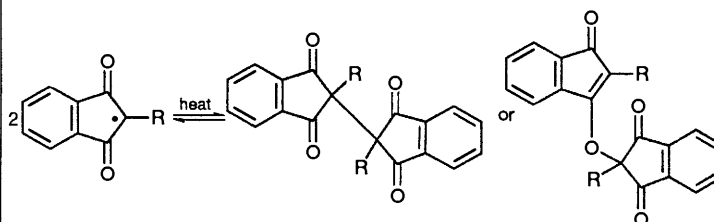
David J. S. Guthrie, Robert F. Geraghty, G. Brent Irvine and Carvell H. Williams



¹H NMR studies show that pQDPFLRFamide and the Asn² and Aib³ analogues can adopt a β -bend predominantly over residues pGlu to Phe in DMSO but over Asp to Leu in aqueous solution

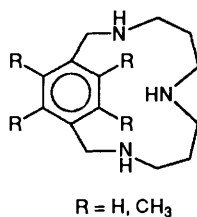
- 1247 **Sterically hindered free radicals. Part 22. Dimerization and EPR spectroscopy of indanedionyl and 9-acylfluorenyl radicals**

Christian Harnack, Wolfgang Krull, Manfred Lehnig, Wilhelm P. Neumann and Antonios K. Zarkadis



1253 Protonation tendencies of azaparacyclophanes.
A thermodynamic and NMR study

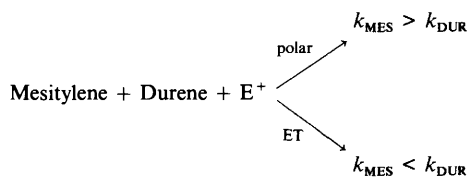
Antonio Bianchi, Beatriz Escuder, Enrique Garcia-España, Santiago V. Luis, Victor Marcelino, Juan F. Miravet and José A. Ramírez



The interaction of hydrogen ions with a series of macrocyclic receptors has been studied in aqueous solution by potentiometry, direct microcalorimetry and ¹H and ¹³C NMR spectroscopy; correlations of the basicity with the atomicity of the macrocycle, the type of chains within the bridge and the nature of the aromatic spacer are advanced

1261 Studies of substrate selectivity in aromatic iodination and other substitution reactions reinforce previous conclusions about the nature of the mechanism of electrophilic aromatic substitutions

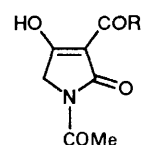
Carlo Galli and Silvia Di Giammarino



Substrate selectivity allows one to distinguish between polar and ET mechanisms of S_EAr

1271 Synthesis, NMR spectroscopic and X-ray crystallographic studies of *N*-acetyl-3-butanoyltetramic acid

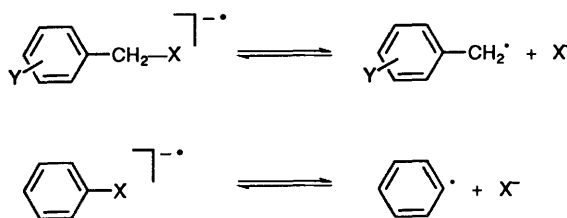
James V. Barkley, John Markopoulos and Olga Markopoulou



The equilibrium between different tautomeric forms of *N*-acetyl-3-butanoyltetramic acid was investigated by ¹H and ¹³C NMR spectroscopy

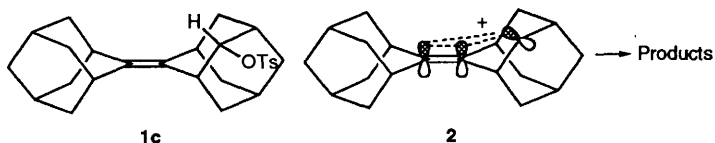
1275 Estimation of bond dissociation Gibbs energies for carbon-halogen bonds in anion radicals of some aryl halides and substituted benzyl halides

Kim Daasbjerg



1279 Observation of an unusually large rate acceleration caused by a homoallylic double bond in the solvolyses of an unstrained secondary adamantyl tosylate

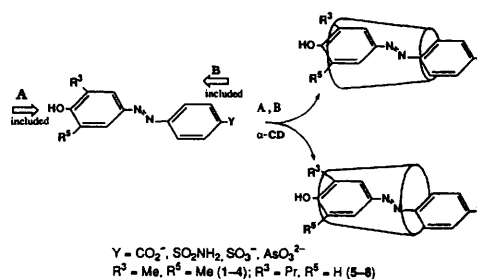
Xicai Huang and Andrew J. Bennet



Solvolysis of **1c** proceeds through a homoallylic stabilized cation **2**
 $k_{1c}/k_{2-AdOTs} = 1.7 \times 10^6$ (25 °C; EtOH)

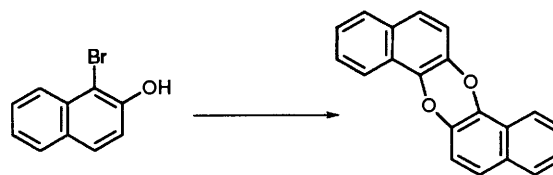
1285 Dynamic aspects in host-guest interactions. Part 2. Directional inclusion reactions of some azo guest molecules with α -cyclodextrin

Noboru Yoshida and Katura Hayashi



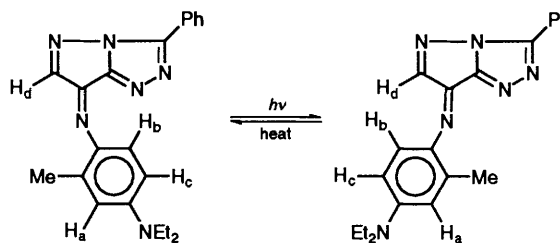
1291 **Self-condensation of 1-bromo-2-naphthol: mechanism of formation of a 1,4-dinaphthodioxin**

Luciano Forlani, Andrea Lugli, Daniele Nanni and Paolo E. Todesco



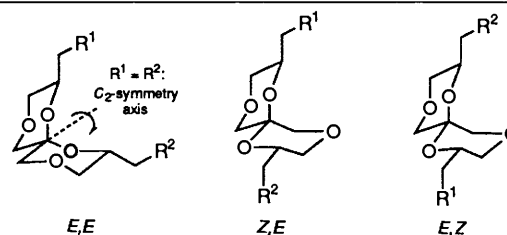
1295 **NMR Study of the configuration and protonation equilibria of a pyrazolotriazole azomethine dye**

Peter Douglas, Christophe Couture, David Clarke, David Reed, Ian H. Sadler and Trevor Wear



1299 **2- And 8-functionalized 1,4,7,10-tetraoxaspiro[5.5]undecanes. Part 4. Conformational study by ^1H and ^{13}C NMR spectroscopy**

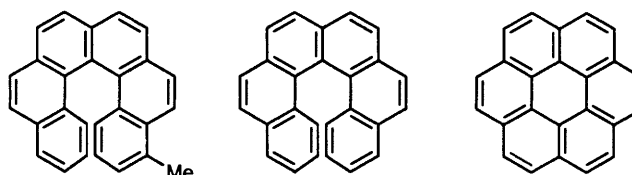
Marielle Lemaire, Georges Jeminet, Annie Cuer, Jean-Gabriel Gourcy and Gérard Dauphin



$\text{R}^1 = \text{R}^2 = \text{NHTs}$, 1; $\text{R}^1 = \text{R}^2 = \text{OH}$, 2; $\text{R}^1 = \text{R}^2 = \text{OCOPr}$, 3; $\text{R}^1 = \text{OH}$, $\text{R}^2 = \text{NHBUt}$, 4; $\text{R}^1 = \text{R}^2$ Z,E = E,Z

1303 **Electrophilic and oxidative chemistry of 4-methyl[6]helicene, [6]helicene and coronene; persistent ion generation in superacid media, gas phase mass spectrometric studies and AM1 calculations**

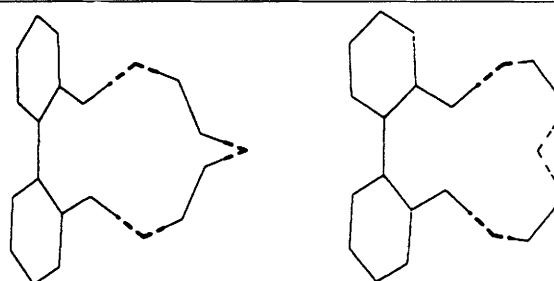
Kenneth K. Laali and John J. Houser



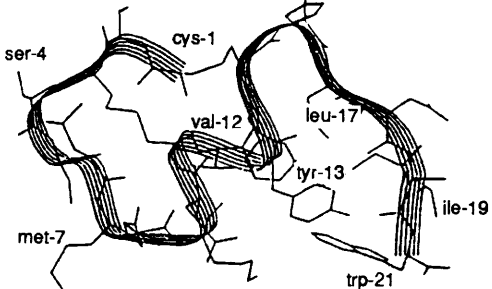
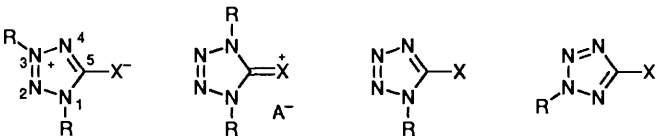
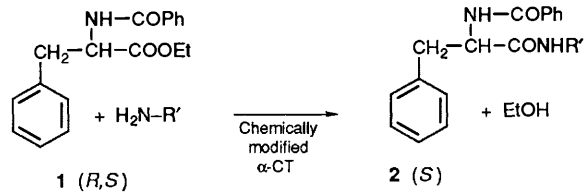
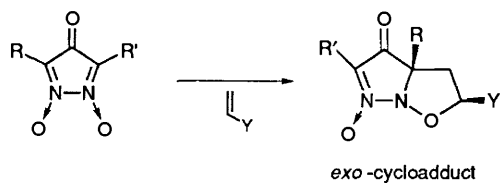
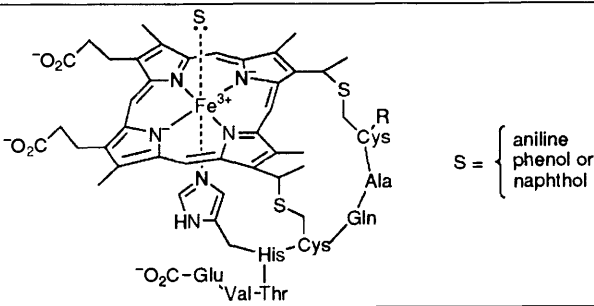
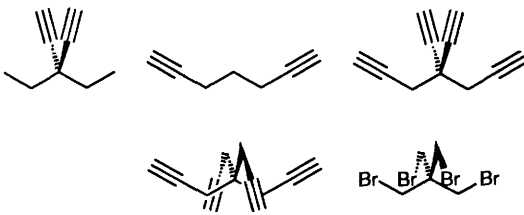
Protonation/oxidation in superacids; reactions with H^+ , MeCO^+ , Me_3Si^+ in the gas phase, and AM1 energies

1309 **New trithia- and dithioxa-macrocycles with biphenyl fused into the backbone: structures, and molecular modelling studies**

Joyce C. Lockhart, David P. Mousley, George A. Forsyth, Francesc Teixidor, Maria P. Almajano, Luis Escriche, Jaume Casabo, Reijo Sillanpää and Raikko Kivekäs

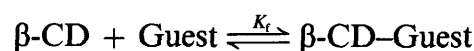


New macrocycles with trithia or dithioxa donors and a biphenyl unit in the skeleton have been synthesised and their structures probed by X-ray crystallography and molecular dynamics simulations

<p>1317 Tertiary structure of endothelin-1 in water by ^1H NMR and molecular dynamics studies</p> <p>Enzio Ragg, Rosanna Mondelli, Sergio Penco, Giorgio Bolis, Luca Baumer and Alberto Guaragna</p>	
<p>1327 A multinuclear NMR study of some mesoionic 1,3-dimethyltetrazoles, 1- and 2-methyltetrazoles and related compounds</p> <p>Wojciech Bocian, Jarosław Jaźwiński, Wiktor Kozmiński, Lech Stefaniak and Graham A. Webb</p>	 <p>^1H, ^{13}C, ^{14}N and ^{15}N NMR spectroscopy</p>
<p>1333 Stereoselectivity of chemically modified α-chymotrypsin and immobilized lipases</p> <p>José Vicente Sinisterra, Emilio Fidel Llama, Carmen del Campo, María José Cabezas, José María Moreno and Miguel Arroyo</p>	
<p>1337 Cycloaddition behaviour of pyrazol-4-one <i>N,N</i>-dioxides toward unsaturated compounds. Stereochemical and mechanistic aspect</p> <p>Masashi Eto, Yasuyuki Yoshitake, Kazunobu Harano and Takuzo Hisano</p>	 <p>exo-cycloadduct</p>
<p>1347 Peroxidatic activity of haem octapeptide complexes with anilines, naphthols and phenols</p> <p>Ian D. Cunningham, John L. Bachelor and John M. Pratt</p>	 <p>S = { aniline, phenol or naphthol }</p>
<p>1351 Sigma-pi interactions in non-conjugated polyalkynes: a photoelectron spectroscopic study</p> <p>Dennis L. Lichtenberger, Lalitha Subramanian, Uwe Bunz and K. Peter C. Vollhardt</p>	 <p>The gas phase conformations of these molecules and the electronic mixing of the alkyne π orbitals with each other and with the σ bond framework are investigated</p>

- 1359 **Binding forces contributing to the complexation of organic molecules with β -cyclodextrin in aqueous solution**

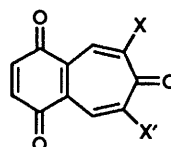
Jung Hag Park and Tae Hwa Nah



Linear solvation energy relationship between K_f and solute properties

- 1363 **X-Ray structures and physical properties of tropone-annulated *p*-benzoquinones substituted with X-Ar groups α to tropone carbonyls and first examples of the trione substituted with an electron-withdrawing group**

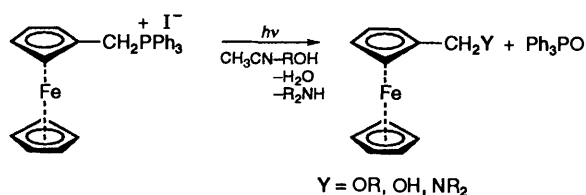
Kimiaki Furuichi, Hitoshi Tada, Akira Itoh, Yasuyo Takeuchi, Masashi Mitoori, Masahiko Kato, Shuji Matsumoto and Masao Hashimoto



X = X': OPh, CH₂Ph
X: SPh X': SOPh

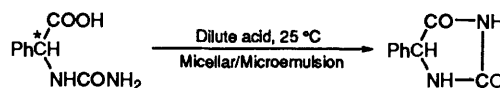
- 1379 **Photochemistry of (ferrocenylmethyl)triphenylphosphonium salts**

Christopher Imrie, Tomasz A. Modro and Carl C. P. Wagener



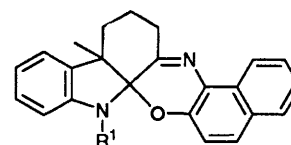
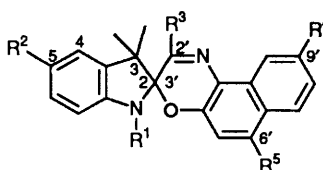
- 1383 **Cyclization and molecular rearrangement under micellar and microemulsion conditions**

Brajesh K. Jha, Ajay S. Chhatre and Bhaskar D. Kulkarni



- 1387 **Studies of relations between molecular structure and photochemical properties of spiro[indoline-2,3'-[1,4]oxazines]**

Meigong Fan, Yangfu Ming, Yongchao Liang, Xinyu Zhang, Sheng Jin, Side Yao and Nianyun Lin

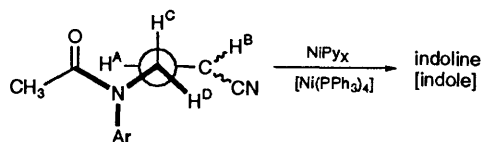


18 R¹ = Me

19 R¹ = Et

- 1393 **Cyclization of *N*-acetyl-*N*-(*ortho*-chlorophenyl)-4-aminobut-2-enitrile with zerovalent nickel complexes: conformational analysis of the *N*-3-cyanoprop-2-enyl chain**

J. Gonzalo Rodriguez and Laureano Canoira



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