

## JOURNAL OF THE CHEMICAL SOCIETY

## Perkin Transactions 2

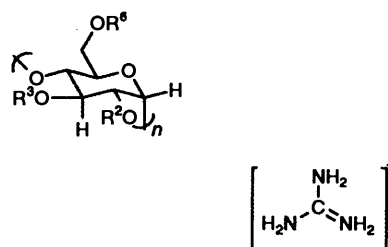
## Physical Organic Chemistry

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## Perkin Communications

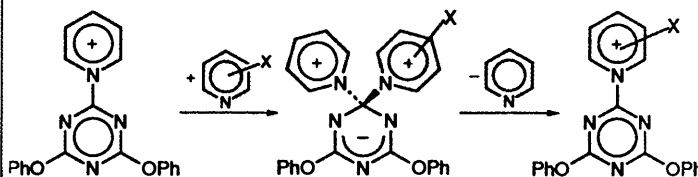
- 2381 **Selective binding and sensing of guanidinium ions by lipophilic cyclodextrins**

Ritu Katakya, Patricia M. Kelly, David Parker and Antonio F. Patti



- 2383 **Timing of bonding changes in fundamental reactions in solution: pyridinolysis of a triazinyl-pyridinium salt**

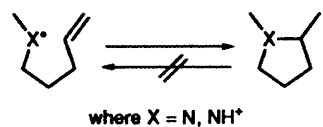
A. Hunter M. Renfrew, John A. Taylor, James M. J. Whitmore and Andrew Williams



The title reaction is demonstrated to involve a Meisenheimer-type intermediate and the full effective charge map is determined for solution states along the reaction pathway

- 2385 **Ab initio study of the homolytic additions of aminyl radicals and ammoniumyl cation radicals to alkenes**

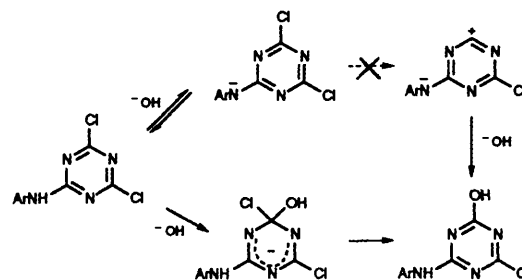
Brendan J. Maxwell, Carl. H. Schiesser, Bruce A. Smart and John Tsanaktsidis



## Articles

- 2389 **Nucleophilic aromatic substitution in heterocycles: alcoholysis and hydrolysis of 2-anilino-4,6-dichloro-1,3,5-triazines**

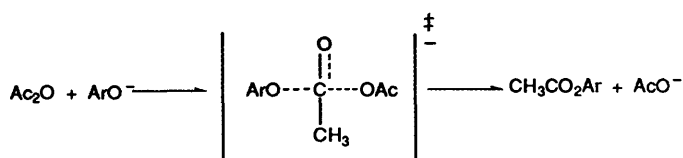
A. Hunter M. Renfrew, John A. Taylor,  
James M. J. Whitmore and Andrew Williams



The alkaline hydrolysis of 2-anilino-4,6-dichloro-1,3,5-triazines involves rate-limiting addition of hydroxide ion to the triazine nucleus; substantial charge accumulation is observed in the triazine ring in the transition state

- 2395 **Kinetics and equilibria of reactions between acetic anhydride and substituted phenolate ions in aqueous and chlorobenzene solutions**

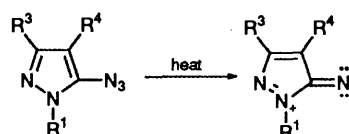
Salem A. Ba-Saif, Antony B. Maude and  
Andrew Williams



Bond formation, measured by Leffler's  $\alpha$  coefficient, is more advanced in chlorobenzene ( $\alpha = 0.62$ ) than in water ( $\alpha = 0.33$ ) for phenolysis of acetic anhydride

- 2401 **Factors affecting rates of thermal decomposition of 5-azidopyrazoles: a comparison with other aromatic azides**

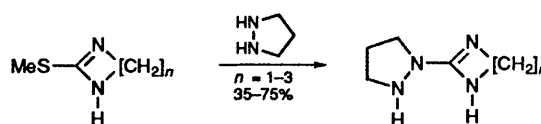
Gerrit L'abbé, Leonard Dyall, Kathleen  
Meersman and Wim Dehaen



The formation of a stabilized nitrene is responsible for the high rates of thermolyses of  $\alpha$ -azidopyrazoles and the absence of neighbouring group effects

- 2407 ***N,N*-Coupled heterobicycles from cyclic hydrazine derivatives. Part 7. Investigations on the synthesis and structure of 1-(*N*<sup>1</sup>,*N*<sup>2</sup>-alkanediyldicarbamimidoyl)pyrazolidine derivatives**

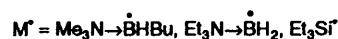
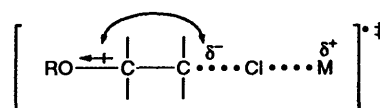
Olaf Morgenstern, Markku Ahlgrén,  
Jouko Vepsäläinen, Peter H. Richter and  
Pirjo Vainiotalo

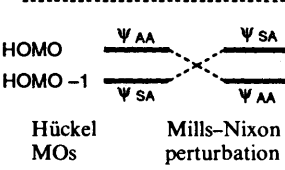
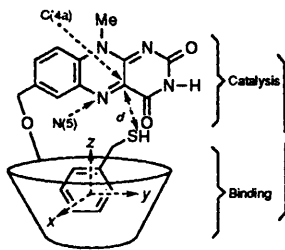
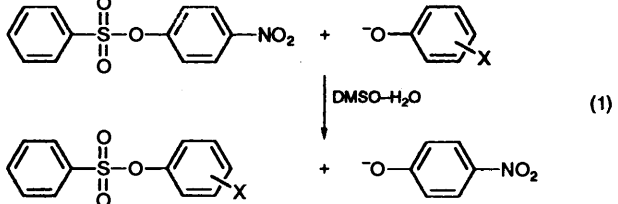
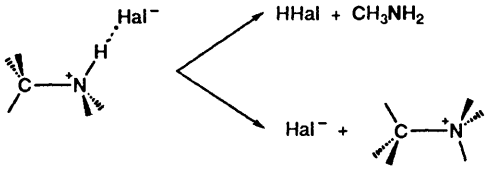
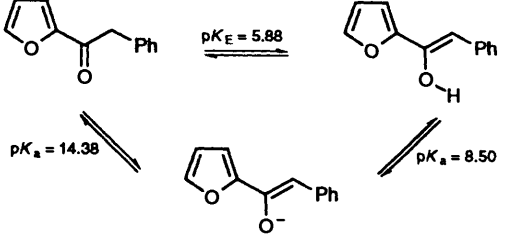


- 2411 **The effects of  $\beta$ -alkoxy substituents on radical reactions: halogen-atom abstraction from alkyl chlorides**

Brian P. Roberts and Andrew J. Steel

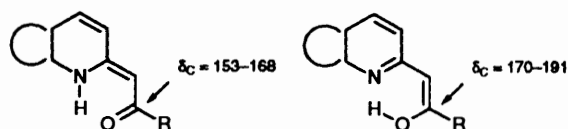
Stabilising electrostatic interaction



<p>2423 <b>The EPR spectrum of the dibenzo[<i>b,h</i>]-biphenylene radical anion and cation: the pairing principle and the Mills–Nixon effect</b></p> <p>Alwyn G. Davies, Georg Gescheidt, Kai M. Ng and Michael K. Shepherd</p>	 <p>HOMO <math>\psi_{AA}</math> <math>\psi_{SA}</math></p> <p>HOMO -1 <math>\psi_{SA}</math> <math>\psi_{AA}</math></p> <p>Hückel MOs Mills-Nixon perturbation</p> <p>Rehybridization, induced by angle strain, interchanges the energy levels of the Hückel HOMO and HOMO - 1 in dibenzo[<i>b,h</i>]biphenylene</p>
<p>2427 <b>The relevance of third-derivative cross interaction coefficients in Hammett-type treatments of nucleophilic substitution reactions</b></p> <p>Dennis N. Kevill and Malcolm J. D'Souza</p>	<p>Using a modified Hammett equation, incorporating second- and third-derivative terms, high probabilities are found for the third-derivative term being statistically insignificant</p>
<p>2431 <b>Flavocyclodextrins as artificial redox enzymes. Part 4. Catalytic reactions of alcohols, aldehydes and thiols</b></p> <p>Hongping Ye, Weida Tong and Valerian T. D'Souza</p>	 <p>Catalysis</p> <p>Binding</p> <p>Artificial Redox Enzyme</p>
<p>2439 <b>Solvent independent transition-state structures. Part III. Sulfonyl transfer reactions</b></p> <p>Richard M. Tarkka, William K. C. Park, Ping Liu, Erwin Buncl and Shmaryahu Hoz</p>	 <p>(1)</p> <p>The novel and traditional Brønsted-type plots are contrasted in a discussion of the TS structure of reaction (1) as the solvent DMSO-H<sub>2</sub>O composition is varied</p>
<p>2445 <b>Semiempirical study of the solvent effect on the Menshutkin reaction</b></p> <p>Uko Maran, Tapani A. Pakkanen and Mati Karelson</p>	 <p><math>\text{HHal} + \text{CH}_3\text{NH}_2</math></p> <p><math>\text{Hal}^- + \text{N}^+</math></p>
<p>2453 <b>Equilibrium constants for ionisation and enolisation of 2-phenylacetylfuran</b></p> <p>Antonella Fontana and Rory A. More O'Ferrall</p>	 <p><math>pK_E = 5.88</math></p> <p><math>pK_a = 14.38</math></p> <p><math>pK_a = 8.50</math></p>

2461  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra of  $\alpha$ -heterocyclic ketones and assignment of keto, enol and enaminone tautomeric structures

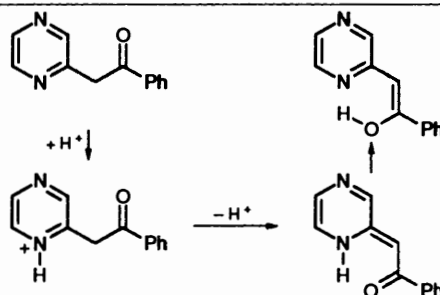
Rory A. More O'Ferrall and Brian A. Murray



$^{13}\text{C}$  chemical shifts of heterocyclic enols and enaminones differ by 20–30 ppm at the oxygen-bound carbon atom

2471 Keto–enol tautomerism of phenacylpyrazine: acid catalysis with protonation at nitrogen

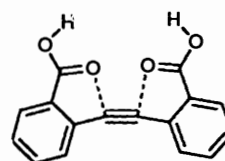
A. R. Edwin Carey, Rory A. More O'Ferrall, Michael G. Murphy and Brian A. Murray



Acid-catalysed enolisation of 2-phenacylpyrazine occurs via an *N*-protonated rather than an *O*-protonated intermediate

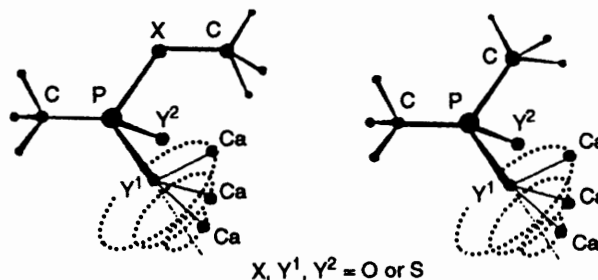
2481 Attractive interactions between an alkyne group and two carbonyl oxygen atoms: the crystal and molecular structure of 2,2'-ethynylenedibenzoic acid at 150 K

Melanie Pilkington, Sidika Tayyip and John D. Wallis



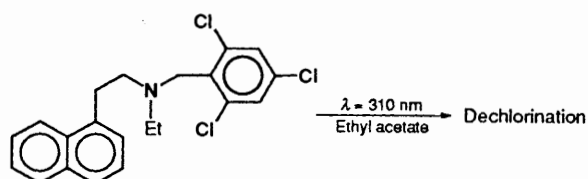
2485 *Ab Initio* studies on organophosphorus compounds. Part 3. Cationic calcium binding to phosphonate and phosphinate monoanions and their sulfur analogues

Jari P. Räsänen, Esko Pohjala and Tapani A. Pakkanen



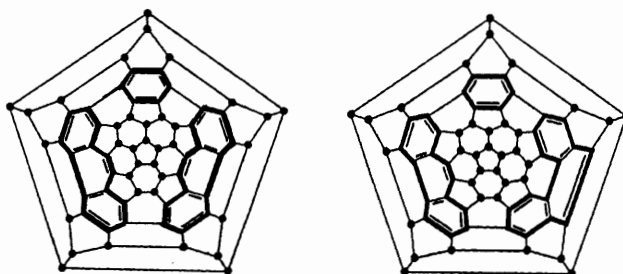
2491 Naphthalene photocatalysed decomposition of chlorobenzenes in exciplex forming systems

Carlos A. Chesta, Vicente Avila, Arnaldo T. Soltermann, Carlos M. Previtali and Juan J. Cosa



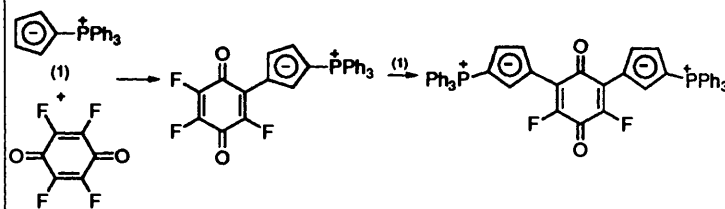
2497  $\text{C}_{70}\text{H}_{36}$  is probably an aromatic compound

Roger Taylor



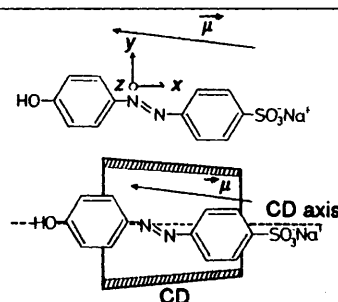
- 2499 Kinetics and mechanism of the addition of triphenylphosphoniocyclopentadienide to tetrahalogeno-*p*-benzoquinones. Part 4. The substitution reactions of fluoranil

Francisco Pérez Pla, C. Dennis Hall, Peter Speers and Juan Palou



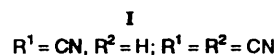
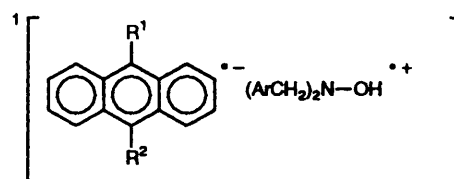
- 2507 Induced circular dichroism spectra of  $\alpha$ -,  $\beta$ - and  $\gamma$ -cyclodextrin complexes with sodium 4'-hydroxy-3'-isopropylazobenzene-4-sulfonate and sodium 4'-hydroxy-3',5'-diisopropylazobenzene-4-sulfonate

Noboru Yoshida, Hiroyuki Yamaguchi and Miwako Higashi



- 2515 Cyanoanthracene-sensitized photooxidations of *N,N*-dibenzylhydroxylamine and its derivatives: free-energy dependence of back electron-transfer rates within geminate radical ion pairs

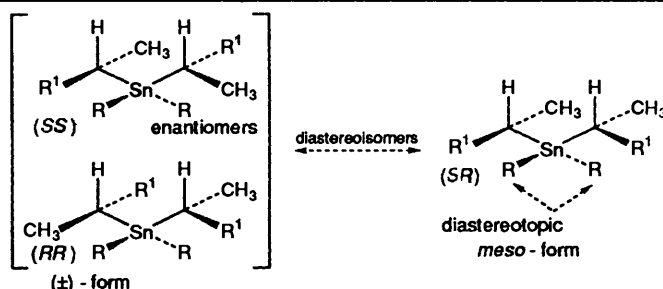
Tadamitsu Sakurai, Mayumi Yokono, Kanako Komiya, Yasuo Masuda and Hiroyasu Inoue



The rates of back electron transfer within the photochemically generated geminate radical ion pairs I show a bell-shaped free-energy dependence

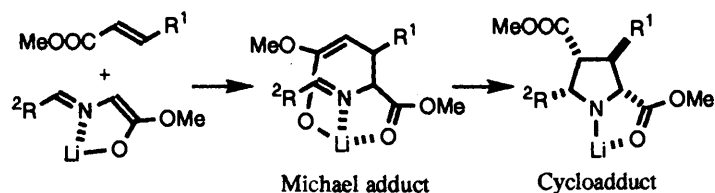
- 2523 Investigations on diastereoisomeric tetraorganotin compounds: the use of <sup>119</sup>Sn NMR spectroscopy for the direct determination of the diastereoisomeric composition

Jens Klein, Solvig Neels and Rolf Borsdorf



- 2525 Semiempirical molecular orbital study on the transition states for the *anti*-selective Michael addition reactions of the lithium *Z*-enolates of *N*-alkylidene glycinate to  $\alpha,\beta$ -unsaturated esters

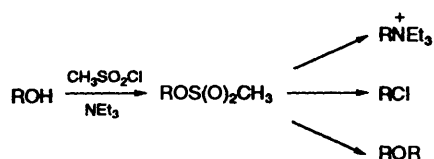
Akira Tatsukawa, Keiko Kawatake, Shuji Kanemasa and Jerzy M. Rudziński



The transition-state structure for the above reaction is analysed by means of semiempirical MO calculations

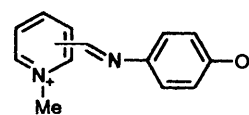
- 2531 Kinetic and spectroscopic characterisation of highly reactive methanesulfonates. Leaving group effects for solvolyses and comments on geminal electronic effects influencing S<sub>N</sub>1 reactivity

T. William Bentley, Manfred Christl, Ralf Kemmer, Gareth Llewellyn and John E. Oakley



2539 Solvato- and halo-chromic behaviour of some 4-[(*N*-methylpyridiniumyl)-methylideneamino]phenolate dyes

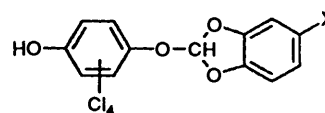
Clodoaldo Machado, Maria da Graça Nascimento and Marcos Caroli Rezende



2-, 3- and 4-substituted

2545 Photoinduced electron transfer reactions of chloranil with benzodioxoles

Bao-Zhen Yan, Zhao-Guo Zhang, Han-Cheng Yuan, Long-Cheng Wang and Jian-Hua Xu



I

X = H, Br, CN, CH<sub>2</sub>CH=CH<sub>2</sub>, NO<sub>2</sub>, COCH<sub>3</sub> etc.

Photoinduced electron transfer reactions of chloranil with benzodioxoles give triaryl orthoformate products I in high yield via an SET mechanism as evidenced by photo-CIDNP studies

2551 One- and two-electron reduction potentials of peroxy radicals and related species

Gábor Merényi, Johan Lind and Lars Engman



2555 The effective 'size' of the tris(trimethylsilyl)silyl group in several molecular environments

Joseph Frey, Etti Schottland, Zvi Rappoport, Dmitry Bravo-Zhivotovskii, Moshe Nakash, Mark Botoshansky, Menahem Kaftory and Yitzhak Apeloig

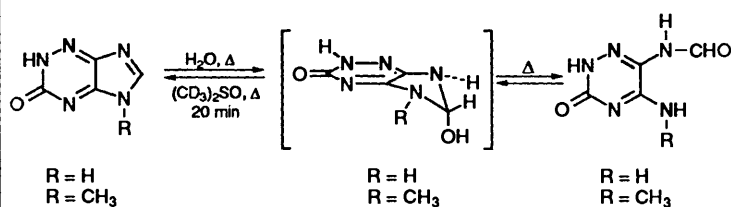


1g

The effective size of the (Me<sub>3</sub>Si)<sub>3</sub>Si group in **1g** and in cyclohexyl derivatives is similar to that of Bu<sup>t</sup>, judged by the X-ray structure of **1g**, the barrier to mesityl rotations in **1g**, by FF calculations and by its *A*-value

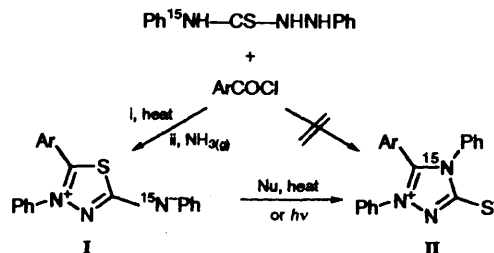
2563 6-Azapurines. Part 3. Covalent  $\sigma$ -adducts of the imidazo[4,5-*e*]-*as*-triazine ring system

Cherng-Chyi Tzeng, Raymond P. Panzica, Jacques Riand and Marie-Thérèse Chenon



2571 **Structural studies on some 1,3,4-thiadiazolium-2-aminides and their rearrangement isomers using  $^{15}\text{N}$  and  $^{13}\text{C}$  NMR**

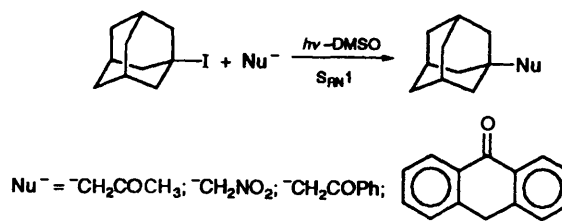
Carlos A. Montanari, John P. B. Sandall, Yukino Miyata and Joseph Miller



The thermodynamic products **II**,  $^1J(^{13}\text{C}-5-^{15}\text{N}-1)$  ca.  $19 \pm 1.5$  Hz, are only obtained by rearrangement of the kinetic products **I**,  $^1J(^{13}\text{C}-2-^{15}\text{N}_{\text{exo}})$  not observed; **I** gives no signal in the  $^{15}\text{N}$  CPMAS NMR spectrum

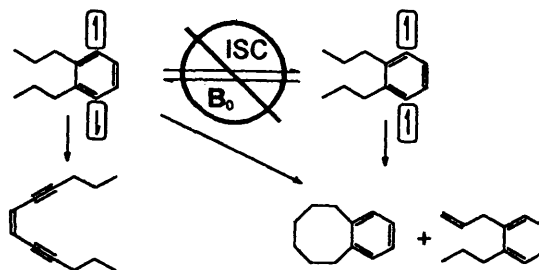
2577 **Reactivity of 1-iodoadamantane with carbanions by the  $\text{S}_{\text{RN}}1$  mechanism**

Roberto A. Rossi, Adriana B. Pierini and Gabriela L. Borosky



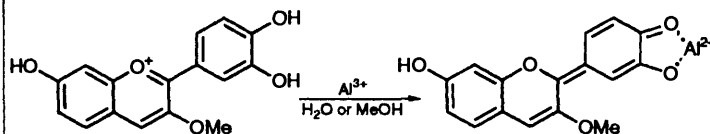
2583 **Absence of intersystem crossing in 1,4-didehydrobenzene**

William B. Lott, Tom J. Evans and Charles B. Grissom



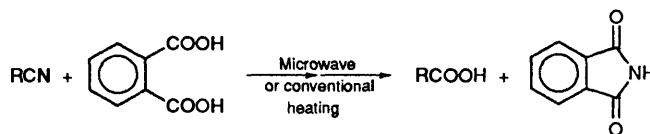
2587 **Kinetic and thermodynamic investigation of the aluminium–anthocyanin complexation in aqueous solution**

Olivier Dangles, Mourad Elhabiri and Raymond Brouillard



2597 **'Dry' hydrolysis of nitriles effected by microwave heating**

Farid Chemat, Martine Poux and Jacques Berlan



No microwave rate enhancement is observed

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xv Conference Diary

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## Forthcoming Articles in *Perkin Transactions 2*

Non-linear optical properties of organic molecules. Part 20. Calculations of the structure, electronic properties and hyperpolarizabilities of donor–acceptor heterocycles containing sulfur, oxygen and nitrogen **J. O. Morley**

Unusual isomer distribution of dinitrobenzenes and nitrophenols formed as side products during the ozone-mediated nitration of benzene with nitrogen dioxide. Further evidence for the alternative mechanism of electrophilic nitration of arenes  
**F. Suzuki and T. Mori**

Ligands which bind weakly to vancomycin: studies by  $^{13}\text{C}$  NMR **C. M. Pearce, U. Gerhard and D. H. Williams**

Complete assignment of the carbon-13 spectrum of vancomycin **C. M. Pearce and D. H. Williams**

Redox properties of 4-substituted aryl methyl chalcogenides in water **M. Jonsson, J. Lind, G. Merényi and T. E. Eriksen**

Acyl transfer reactions mediated by cyclodextrins. The reaction of external nucleophiles with encapsulated alkanoate esters of varying chain length **T. A. Gadosy and O. S. Tee**

Stereoelectronic requirements of benzamide 5HT<sub>3</sub> antagonists. Comparison with D<sub>2</sub> antidopaminergic analogues  
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