

Physical Organic Chemistry

CONTENTS

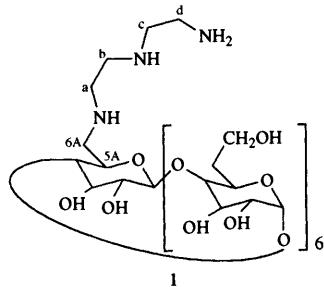
Articles

- 1785 Functionalized β -cyclodextrins: thermodynamic studies and NMR titration of 6-diethylene-triamine derivative**

Vincenzo Cucinotta, Franca D'Alessandro, Giuseppe Impellizzeri, Giuseppe Maccarrone, Enrico Rizzarelli and Graziella Vecchio

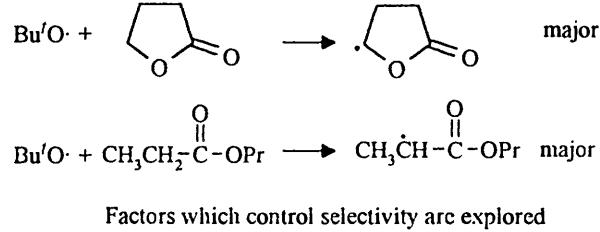


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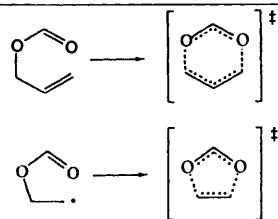
- 1789 Application of EPR spectroscopy to the determination of the rates of reaction and selectivity of attack of the *tert*-butoxyl radical on esters: the interplay of electronic, polar, steric and stereoelectronic factors**

John E. Bennett, Bruce C. Gilbert, Sara Lawrence, Adrian C. Whitwood and Andrew J. Holmes



- 1797 Acyloxy-shifts in open and closed shell systems—intramolecular nucleophilic substitution reactions in disguise**

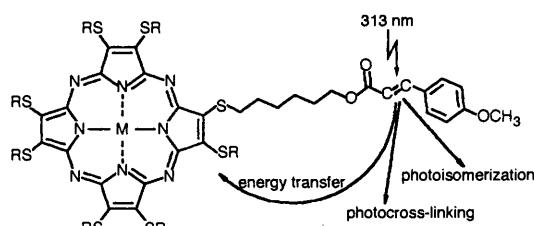
Hendrik Zipse



The analogy between vinyl and methylene groups can be used to connect the world of open and closed shell reactivity

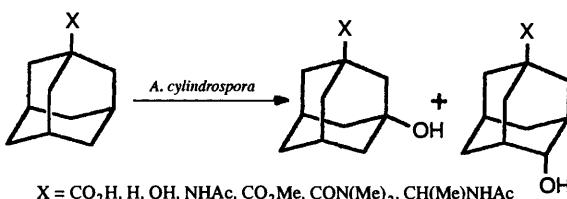
- 1801 Synthesis and photochemical properties of octacinnamoyl-substituted tetraazaporphyrins**

H. Eichhorn, M. Rutloh, D. Wöhrle and J. Stumpf



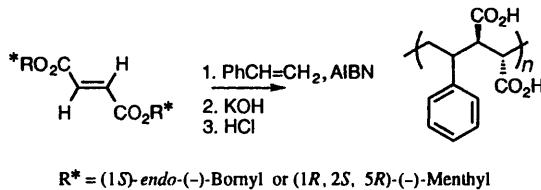
1811 Site selective oxidation of tricyclo-[3.3.1.1^{3,7}]decane (adamantane) and some of its derivatives using fungi of the genus *Absidia*

Colin H. Ridyard, Roger A. Whittaker, Stanley D. Higgins, Stanley M. Roberts, Andrew J. Willets, Patrick D. Bailey and Georgina M. Rosair



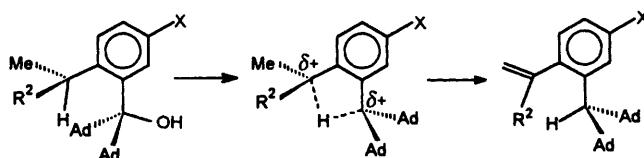
1821 Use of readily available monomers in the synthesis of vinyl copolymers with optical activity arising from the configuration of stereogenic carbon atoms in the main chain

Irene H. Donnelly, Peter Kambouris, Derek C. Nonhebel, Thomas Rohr and David C. Sherrington



1831 1,4-Hydride shifts in *ortho*-alkyl-substituted di(1-adamantyl)benzyl cations: an NMR spectroscopic and X-ray crystallographic study

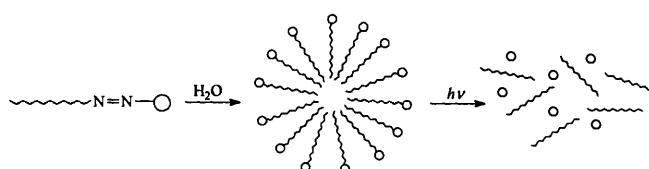
John S. Lomas and Jacqueline Vaissermann



Intramolecular H-shift is faster than intermolecular reaction with TES

1837 Synthesis, characterization and applications of azo-containing photodestructible surfactants

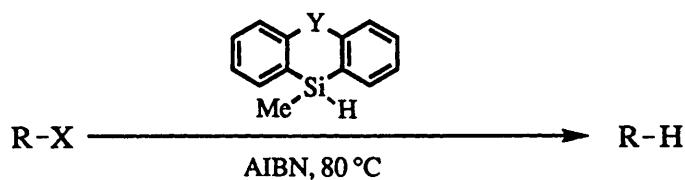
Ian R. Dunkin, Andreas Gittinger, David C. Sherrington and Paul Whittaker



Azo-containing surfactant micelles destroyed by UV light

1843 9,10-Dihydro-9-sila-10-heteroanthracenes as new radical-based reducing agents

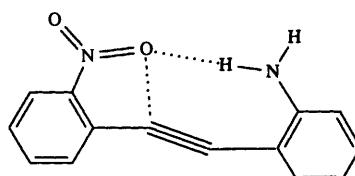
Makoto Oba, Yoko Kawahara, Ryo Yamada, Hidekata Mizuta and Kozaburo Nishiyama



$\text{X}=\text{Cl, Br, OCSNPh, OCSNHAc, OCSOC}_6\text{H}_4\text{-4-F}$
 $\text{Y=SiHMe, SiHPh, SiMe}_2, \text{SnMe}_2, \text{O, S}$

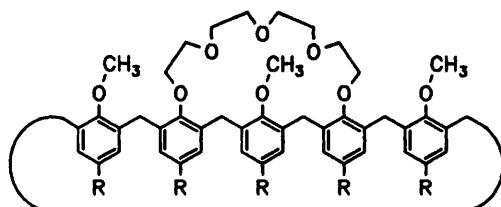
1849 Geometry distorting intramolecular interactions to an alkyne group in 1-(2-amino-phenyl)-2-(2-nitrophenyl)ethyne: a joint experimental-theoretical study

Melanie Pilkington, John D. Wallis, Garry T. Smith and Judith A. K. Howard



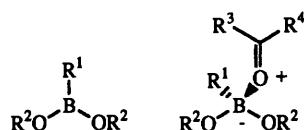
CONTENTS

- ## 1855 Crown ether derivatives of calix[5]arenes: synthesis and complexation properties



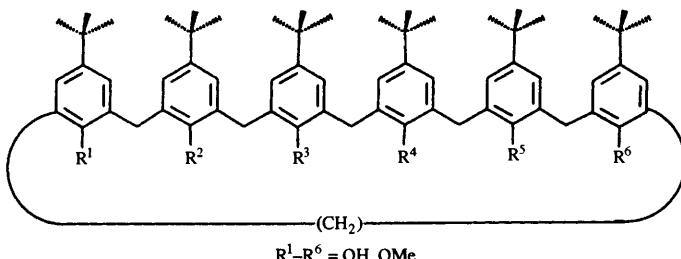
Fran oise Arnaud-Neu, Ralf Arnecke,
Volker B hmer, Stefano Fanni, James L. M.
Gordon, Marie-Jos  Schwing-Weill and
Walter Vogt

- ## 1861 Force field parameters for the boronate function and their carbonyl complexes and application to modelling boronate esters



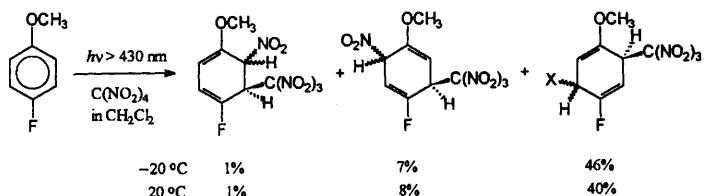
Jeffrey J. James and Andrew Whiting

- ## 1869 Spectroscopic studies of hydrogen-bond structures and dynamics of partially methylated *p*-*tert*-butylcalix[6]arenes



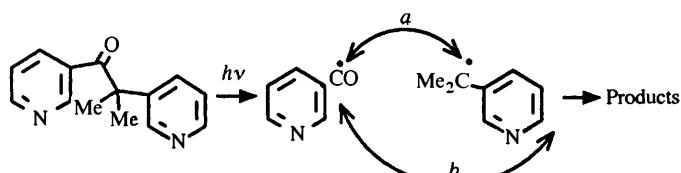
Rob G. Janssen, Willem Verboom, Bert T. G. Lutz, John H. van der Maas, Myrek Maczka, John P. M. van Duynhoven and David N. Reinhoudt

- 1877 Photochemical nitration by tetrannitromethane.
Part 36. Adduct formation in the photochemical
reactions of 4-fluoroanisole and 4-fluoro-3-
methylanisole**



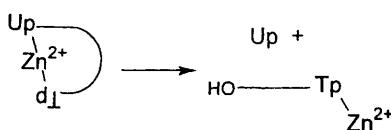
Craig P. Butts, Lennart Eberson, Michael P. Hartshorn and Ward T. Robinson

- 1889 The photochemistry of metyrapone



Elisa Fasani, Mariella Mella, Sandra Monti,
Salvatore Sortino and Angelo Albini

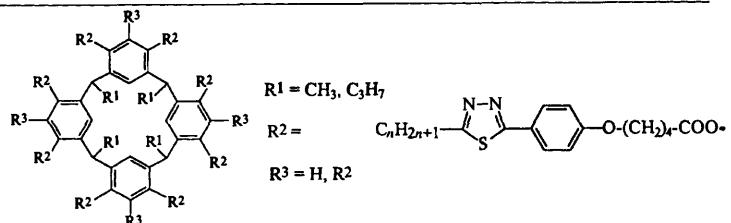
- 1895 Acceleration of the Zn²⁺-promoted phosphodiester hydrolysis of oligonucleotides by the 3'-terminal monophosphate group: intrastrand participation over several nucleoside units



Satu Kuusela, Andrei Guzaev and
Harri Lönnberg

1901 Mesomorphic properties and monolayer behaviour of novel liquid crystalline *exo*-calix[4]arene derivatives

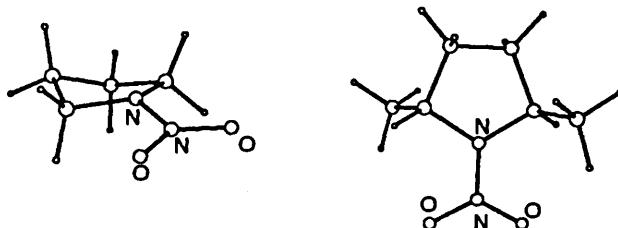
Hansjörg Budig, Siegmar Diele,
Reinhard Paschke, Dieter Ströhle and
Carsten Tschiesske



Calix[4]arene derivatives incorporating calamitic 2-phenylthiadiazole units can form smectic liquid crystalline phases and monomolecular layers at the air-water interface

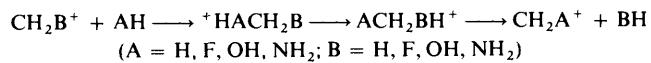
1907 Conformation and circular dichroism of some *N*-nitropyrrolidines

Gennadii V. Shustov, Masood Parvez and
Arvi Rauk



1915 Nucleophilic addition/elimination on substituted methyl cations. Analysis of factors that affect thermochemistry and barrier heights

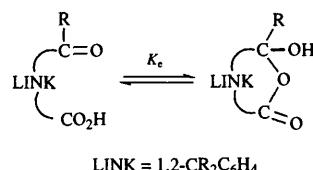
Einar Uggerud



A balance between the p-donor capabilities of the groups A and B determine both well depths and barrier heights in the above reactions

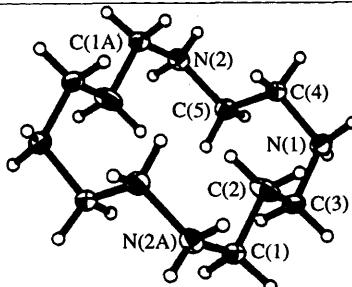
1921 Ring-chain tautomerism. Part 8. Substituted 2-(2-oxopropyl) and 2-(2-oxo-2-phenylethyl)-benzoic and 2-(2-acetyl and 2-benzoylphenyl)-acetic acids

Keith Bowden and Jane M. Byrne



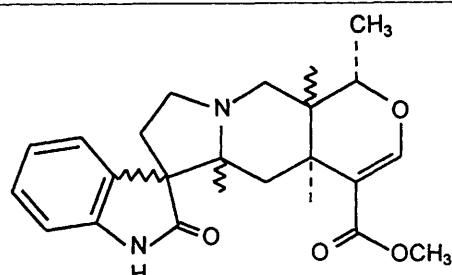
1925 The unusual protonation constants of cyclam. A potentiometric, crystallographic and molecular mechanics study

Robert D. Hancock, Ramunas J. Motekaitis,
Jeremiah Mashishi, Ignacy Cukrowski, Joseph
H. Reibenspies and Arthur E. Martell



1931 Analysis of the kinetics of isomerization of spiro oxindole alkaloids

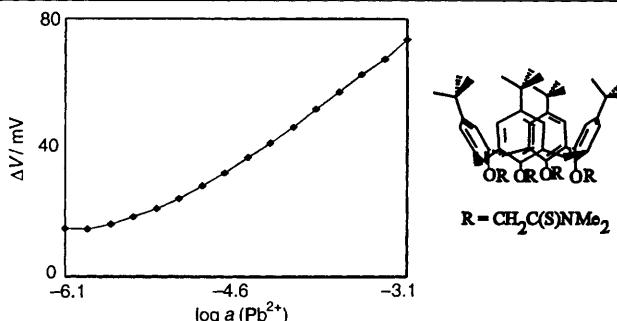
Gerhard Laus, Dagmar Brössner, Gilbert
Senn and Klaus Wurst



CONTENTS

1937 Polysiloxane based CHEMFETs for the detection of heavy metal ions

Ronny J. W. Lugtenberg, Martijn M. G. Antonisse, Richard J. M. Egberink, Johan F. J. Engbersen and David N. Reinhoudt



1943 Nitration of dimethoxybenzenes, mesitylene and toluene with nitric acid and mixed acid studied by ^{15}N -CIDNP

Free radical processes exclusively occur during nitration of *o*-dimethoxybenzene and are side-reactions during nitration of mesitylene and toluene

Manfred Lehnig

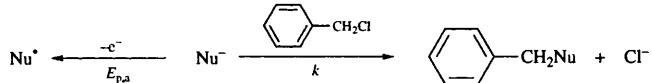
1949 Conformational analysis. Part 28. OH . . . F hydrogen bonding and the conformation of *trans*-2-fluorocyclohexanol

Raymond J. Abraham, Timothy A. D. Smith and W. Anthony Thomas



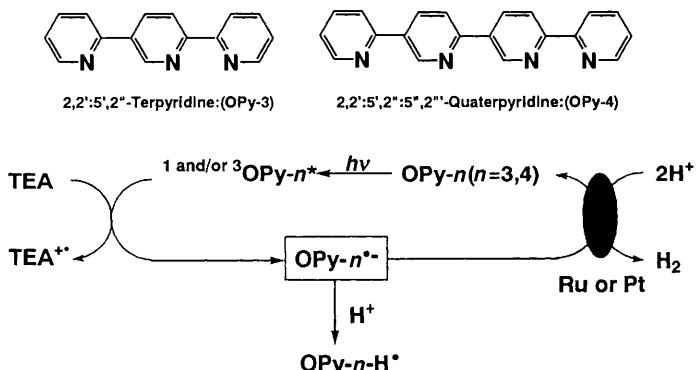
1957 Oxidation potential as a measure of the reactivity of anionic nucleophiles. Behaviour of different classes of nucleophiles

Murat E. Niyazymbetov, Zhou Rongfeng and Dennis H. Evans



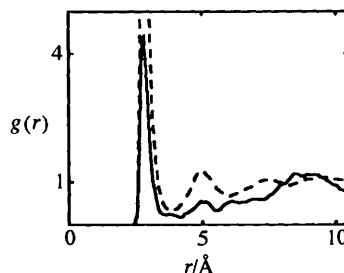
1963 Synthesis of 2,2':5',2''-terpyridine and 2,2':5',2'';5'',2'''-quaterpyridine and their photocatalysis of the reduction of water

Shozo Yanagida, Tomoyuki Ogata, Yasuhiro Kuwana, Yuji Wada, Kei Murakoshi, Akito Ishida, Setsuo Takamuku, Mitsuhiro Kusaba and Nobuaki Nakashima



1971 Interactions between metal cations and the ionophore lasalocid. Part 14. Structure of lasalocid–alkali metal cation complex salts in methanol from NMR spectroscopy and computational experiments

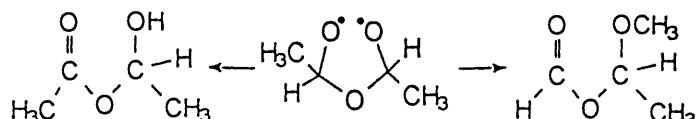
Patrice Malfreyt, Rachid Lyazghi, Gérard Dauphin, Yves Pascal and Jean Juillard



$\text{Rb}^+ \cdots \text{O}$ (methanol) radial distribution functions for the cation free (---) and in its lasalocid complex salt (—)

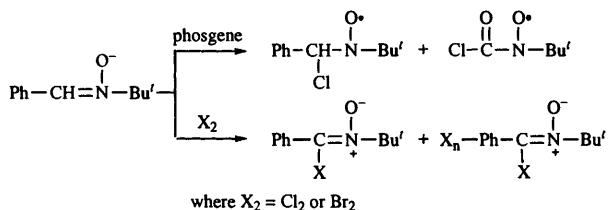
1981 Laser-photosensitized homogeneous decomposition of 3,5-dimethyl-1,2,4-trioxolane: the evidence for intermediacy of products of rearrangement

Lavrenti Khachatryan, Radek Fajgar, Yehuda Haas and Josef Pola



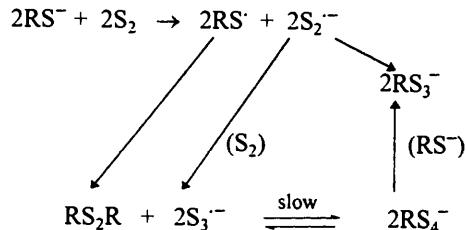
1985 EPR and mass spectroscopic identification of radical adducts produced spontaneously from reactions of phosgene, chlorine gas and bromine with *C*-phenyl *N*-*tert*-butyl nitrone (PBN)

Hong Sang, Edward G. Janzen, Coit M. DuBose, Edwin J. Geels and J. Lee Poyer



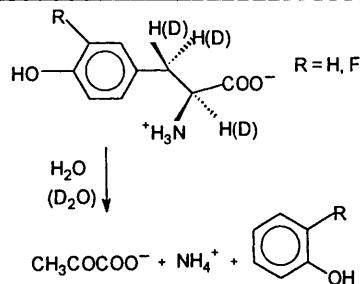
1993 Formation and scission of the sulfur–sulfur bond: a new approach to reactions between sulfur/polysulfide ions and thiolate ions/disulfides in *N,N*-dimethylacetamide

Gérard Bosser, Meriem Anouti and Jacky Paris



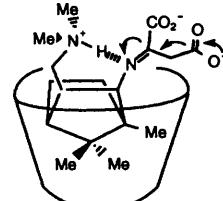
2001 Mechanism of catalysis by tyrosine phenol lyase from *Erwinia herbicola*. Multiple kinetic isotope effects for the reactions with adequate substrates

Nikolai G. Faleev, Svetlana N. Spirina, Tatyana V. Demidkina and Robert S. Phillips



2005 Inclusion effects of cyclodextrins on the catalytic activity of 3-*endo*-dimethylaminomethyl-1,7,7-trimethylnorbornan-2-*endo*-amine for the decarboxylation of oxalacetate

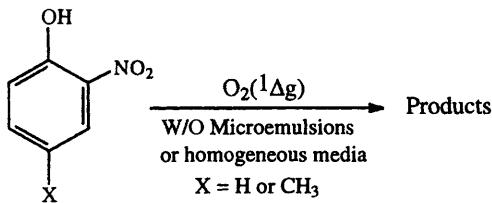
Kenji Ogino, Hideki Azuma, Hiroki Tamiya and Waichiro Tagaki



The title diamine has a high catalytic activity for the decarboxylation of oxalacetate by inclusion into the β -CD cavity

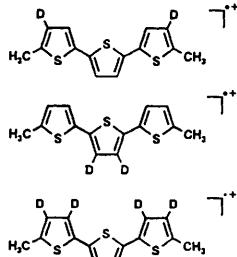
2009 Singlet molecular oxygen-mediated photooxidation of nitrophenolic compounds in water-in-oil microemulsions. A kinetic study

Claudio D. Borsarelli, Edgardo N. Durantini and Norman A. Garcia



2015 EPR investigations of β-deuteriated 5,5"-dimethyl-2,2':5',2"-terthiophenes

Günnar Engelmann, Reinhard Stößer, Gerhard Koßmehl, Werner Jugelt and Hans-Peter Welzel



The structural assignment of the hyperfine coupling constants of terthiophene radical cations takes place by deuterated compounds

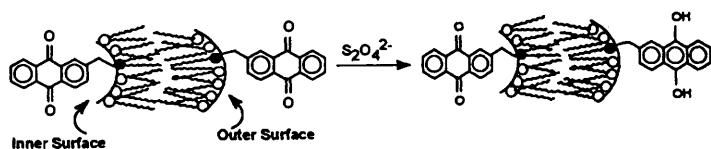
2021 Dialkylaminopyridine catalysed esterolysis of *p*-nitrophenyl alkanoates in different cationic microemulsions

Santanu Bhattacharya and Karnam Snehalatha

Increase in ester hydrophobicity leads to greater resistance in their hydrolysis by dialkylaminopyridine in microemulsions

2027 Synthesis, redox and electrochemical properties of new anthraquinone-attached micelle- and vesicle-forming cationic amphiphiles

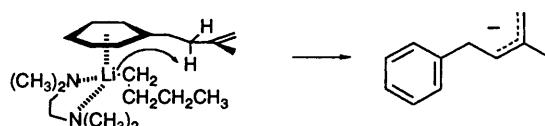
Santanu Bhattacharya and Marappan Subramanian



Vesicle-bound anthraquinones can be differentiated kinetically between outer and inner surfaces

2035 Dianions of 4-phenylbut-1-ene. Evidence for complex-induced proximity effects in the double metallation of hydrocarbons

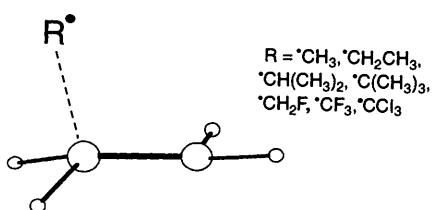
Nancy S. Mills and C. Channing Ruud



CIPE promotes allylic proton abstraction rather than benzylic proton abstraction

2041 Theoretical study of the addition of alkyl and halogenoalkyl radicals to the ethylene double bond: a comparison between Hartree–Fock, perturbation theory and density functional theory

Andrea Bottoni



AUTHOR INDEX

- Abraham, Raymond J., 1949
Albini, Angelo, 1889
Anouti, Meriem, 1993
Antonisse, Martijn M. G., 1937
Arnaud-Neu, Françoise, 1855
Arnecke, Ralf, 1855
Azuma, Hideki, 2005
Bailey, Patrick D., 1811
Bennett, John E., 1789
Bhattacharya, Santanu, 2021,
2027
Böhmer, Volker, 1855
Borsarelli, Claudio D., 2009
Bossé, Gérard, 1993
Bottoni, Andrea, 2041
Bowden, Keith, 1921
Brössner, Dagmar, 1931
Budig, Hansjörg, 1901
Butts, Craig P., 1877
Byrne, Jane M., 1921
Cukrowski, Ignacy, 1925
Cucinotta, Vincenzo, 1785
D'Alessandro, Franca, 1785
Dauphin, Gérard, 1971
Demidkina, Tatyana V., 2001
Diele, Siegmund, 1901
Donnelly, Irene H., 1821
DuBose, Coit M., 1985
Dunkin, Ian R. 1837
Durantini, Edgardo N., 2009
Eberson, Lennart, 1877
Egberink, Richard J. M., 1937
Eichhorn, H., 1801
Engbersen, Johan F. J., 1937
Engelmann, Gunnar, 2015
Evans, Dennis H., 1957
Fajgar, Radek, 1981
Faleev, Nikolai G., 2001
Fanni, Stefano, 1855
Fasani, Elisa, 1889
García, Norman A., 2009
Geels, Edwin J., 1985
Gilbert, Bruce C., 1789
Gittinger, Andreas, 1837
Gordon, James L. M., 1855
Guzaev, Andrei, 1895
Haas, Yehuda, 1981
Hancock, Robert D., 1925
Hartshorn, Michael P., 1877
Higgins, Stanley D., 1811
Holmes, Andrew J., 1789
Howard, Judith A. K., 1849
Impellizzeri, Giuseppe, 1785
Ishida, Akito, 1963
James, Jeffrey J., 1861
Janssen, Rob G., 1869
Janzen, Edward G., 1985
Jugelt, Werner, 2015
Juillard, Jean, 1971
Kambouris, Peter, 1821
Kawahara, Yoko, 1843
Khachatryan, Lavrenti, 1981
Koßmehl, Gerhard, 2015
Kusaba, Mitsuhiro, 1963
Kuusela, Satu, 1895
Kuwana, Yasuhiro, 1963
Laus, Gerhard, 1931
Lawrence, Sara, 1789
Lehnig, Manfred, 1943
Lomas, John S., 1831
Lönnberg, Harri, 1895
Lugtenberg, Ronny J. W., 1937
Lutz, Bert T. G., 1869
Lyazghi, Rachid, 1971
Maccarrone, Giuseppe, 1785
Maczka, Myrek, 1869
Malfreyt, Patrice, 1971
Martell, Arthur E., 1925
Mashishi, Jeremiah, 1925
Mella, Mariella, 1889
Mills, Nancy S., 2035
Mizuta, Hidetaka, 1843
Monti, Sandra, 1889
Motekaitis, Ramunas J., 1925
Murakoshi, Kei, 1963
Nakashima, Nobuaki, 1963
Nishiyama, Kozaburo, 1843
Niyazymbetov, Murat E., 1957
Nonhebel, Derek C., 1821
Oba, Makoto, 1843
Ogata, Tomoyuki, 1963
Ogino, Kenji, 2005
Paris, Jacky, 1993
Parvez, Masood, 1907
Pascal, Yves, 1971
Paschke, Reinhard, 1901
Phillips, Robert S., 2001
Pilkington, Melanie, 1849
Pola, Josef, 1981
Poyer, J. Lee, 1985
Rauk, Arvi, 1907
Reibenspies, Joseph H., 1925
Reinhoudt, David N., 1869,
1937
Ridyard, Colin H., 1811
Rizzarelli, Enrico, 1785
Roberts, Stanley M., 1811
Robinson, Ward T., 1877
Rohr, Thomas, 1821
Rongfeng, Zhou, 1957
Rosair, Georgina M., 1811
Rutloh, M., 1801
Ruud, C. Channing, 2035
Sang, Hong, 1985
Schwing-Weill, Marie-José,
1855
Senn, Gilbert, 1931
Sherrington, David C., 1821,
1837
Shustov, Gennadii V., 1907
Smith, Garry T., 1849
Smith, Timothy A. D., 1949
Snehalatha, Karnam, 2021
Sortino, Salvatore, 1889
Spirina, Svetlana N., 2001
Stößer, Reinhard, 2015
Ströhl, Dieter, 1901
Stumpe, J., 1801
Subramanian, Marappan, 2027
Tagaki, Waichiro, 2005
Takamuku, Setsuo, 1963
Tamiya, Hiroki, 2005
Thomas, W. Anthony, 1949
Tschiesske, Carsten, 1901
Uggerud, Einar, 1915
Vaissermann, Jacqueline,
1831
van der Maas, John H., 1869
van Duynhoven, John P. M.,
1869
Vecchio, Graziella, 1785
Verboom, Willem, 1869
Vogt, Walter, 1855
Wada, Yuji, 1963
Wallis, John D., 1849
Welzel, Hans-Peter, 2015
Whiting, Andrew, 1861
Whittaker, Paul, 1837
Whittaker, Roger A., 1811
Whitwood, Adrian C., 1789
Willets, Andrew J., 1811
Wöhrle, D., 1801
Wurst, Klaus, 1931
Yamada, Ryo, 1843
Yanagida, Shozo, 1963
Zipse, Hendrik, 1797

Submission of chemical structure diagrams

The range of file formats accepted by the Royal Society of Chemistry now includes ISIS/Draw (exported as .tgf) as well as ChemDraw and ChemWindow (exported as .chm). Authors should supply structure diagrams on disk in one of these formats if at all possible.

NOTE: An asterisk in the heading of each paper indicates the author who is
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Forthcoming Articles in *Perkin Transactions 2*

Kinetics and mechanism of the basic hydrolysis of nitrosoureas
S. Amado, L. García-Río, J.R. Leis and A. Ríos

Theoretical studies on long-range substituent effects in the reduction of 7-norbornanones
G.M. Keserü, Z. Kovári and G. Náray-Szabó

Conformational study of six-membered phostones. *cis*- and *trans*-3-Methoxycarbonyl-2-methoxy-2-oxo-1,2-oxaphosphorinane
M.K. Tasz, O.P. Rodriguez, S.E. Cremer, M.S. Hussain and M.-ul-Haque

Oxidation of 2,3-dimethylindole by peroxyphosphates
R. Ghanem, C. Carmona, M.A. Muñoz, P. Guardado and M. Balón

Paramagnetic intermediates in the photolysis of 2-methylpropanoyltripropylstannane studied by means of multinuclear CIDNP
A.I. Kruppa, M.B. Taraban, S.A. Svarovsky and T.V. Leshina

Flash vacuum thermolysis of 5-(1-chloroethenyl)acenaphthene. A short synthesis of pyracylene and its behaviour under high temperature conditions
M. Sarobe, S. Flink, L.W. Jenneskens, J.W. Zwinkker and J. Wesseling

The *D* parameter (zero-field splitting) as a direct measure of structural and electronic effects in localized triplet 1,3-diradicals
W. Adam, H.M. Harrer, T. Heidenfelder, T. Kammel, F. Kita, W.M. Nau and C. Sahin

EPR studies of the formation and transformation of isomeric radicals [C₃H₅O][·]: Rearrangement of the allyloxy radical in non-aqueous solution involving a formal 1,2-hydrogen atom shift promoted by alcohols
P.E. Elford and B.P. Roberts

An *ab initio* study of some free-radical homolytic substitution reactions at silicon, germanium and tin
C.H. Schiesser, M.L. Styles and L.M. Wild

The visible spectrum of dinitrogen trioxide in aqueous solution
A.M.M. Doherty, N. Haine, E. Jones and G. Stedman

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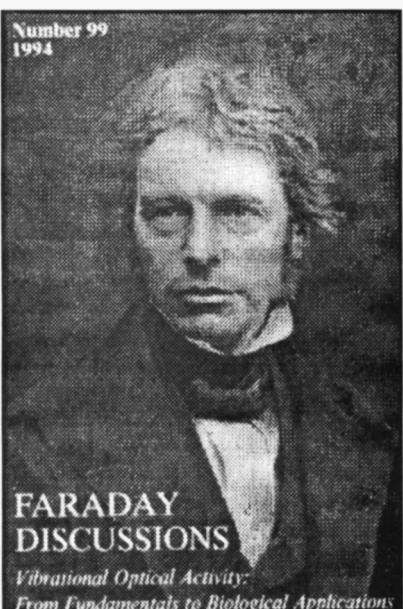
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