

JOURNAL OF THE CHEMICAL SOCIETY

Chemical Communications

Number 16

1990

CONTENTS

- 1069 A Controlled Balance between Ionic and Radical Pathways in Reactions of Tributyltin Hydride **John A. Murphy, Michael S. Sherburn, Julia M. Dickinson, Chris Goodman**
- 1070 Application of New Optically Pure Ketene Equivalents Derived from Tartaric Acids to the Total, Asymmetric Syntheses of (+)-6-Deoxycastanospermine and (+)-6-Deoxy-6-fluorocastanospermine **Jean-Louis Reymond, Pierre Vogel**
- 1072 Unexpected Acid-catalysed Rearrangement of Certain 3-(Arylthio)indoles to 2-(2-Aminophenyl)benzothiophenes **Pierre Hamel, Yves Girard, Joseph G. Atkinson, Michael A. Bernstein**
- 1074 A Long-range Intramolecular Functionalization by Alkoxy Radicals: a Long-range Intramolecular Oxygenation of C(15) of the Androstane Skeleton **Kazuhiko Orito, Masaru Ohto, Hiroshi Suginome**
- 1076 A Wagner–Meerwein Rearrangement of the Cholestane Skeleton induced by a Long-range Intramolecular Hydrogen Abstraction by Alkoxy Radicals; the First Example of Long-range Intramolecular Addition of an Alkoxy Radical to a Carbon–Carbon Double Bond **Kazuhiko Orito, Masaru Ohto, Hiroshi Suginome**
- 1079 A Novel Synthesis of Protoanemonin by the Catalytic Vapour-phase Oxidation of Silvan **Irina Iovel, Yuri Goldberg, Mariya Shymanska**
- 1080 2-Bromomethylprop-2-en-1-yl Acetate; Synthesis and Applications **Göran Magnusson, Fritiof Lindqvist**
- 1081 Dual Luminescence from a Mixed-metal Complex Containing Rhenium(I) and Ruthenium(II) Photochromophores **Shawn Van Wallendael, D. Paul Rillema**
- 1083 Calix[4]arene as a Polyoxo Matrix for Functionalizable and Reducible Niobium(V) and Tantalum(V) Chlorides and Oxochlorides **Fabio Corazza, Carlo Floriani, Angiola Chiesi-Villa, Carlo Guastini**
- 1084 Phosphonium Cascade Molecules **Kasthuri Rengan, Robert Engel**
- 1085 Nucleophilic Addition Vinylketene- and Vinylketenimine (Allenylideneamine)tricarbonyliron(0) Complexes **Lawrence Hill, Christopher J. Richards, Susan E. Thomas**
- 1087 Diastereoselective Radical Addition to Derivatives of Dehydroalanine and of Dehydrolactic Acid **Athelstan L. J. Beckwith, Christina L. L. Chai**
- 1088 Phosphine Complexes of Lanthanum and Lutetium **Michael D. Fryzuk, T. S. Haddad**
- 1090 ‘Caging’ of and Catalysis by a Complex inside a Polymer Matrix **A. Patchornik, Y. Ben-David, D. Milstein**
- 1091 Lipase-catalysed Enantioselective Ring-opening of Oxazol-5(4H)-ones coupled with Partial *in situ* Racemisation of the Less Reactive Isomer **Hanamanthsa S. Bevinakatti, Ravindra V. Newadkar, Ankur A. Banerji**
- 1093 Colourless Nonlinear Optical D- π -A Polymers with Sulphones as Electron Acceptors **S. Nijhuis, G. L. J. A. Rikken, E. E. Havinga, W. ten Hoeve, H. Wynberg, E. W. Meijer**
- 1094 Role of Valency of Copper in the Direct Decomposition of Nitrogen Monoxide over Well Characterized $\text{La}_{2x}\text{A}'_x\text{Cu}_{1-y}\text{B}'_y\text{O}_4$ **Hiroyuki Yasuda, Noritaka Mizuno, Makoto Misono**
- 1096 Theoretical Study on the Unusual Effect of Phenyl Substituent on Second-order Hyperpolarizability **Masato Kodaka, Toshio Fukaya, Katsumi Yonemoto, Isao Shibuya**
- 1098 Selective Carbonylation of Propane in Supercritical Media *via* Hydride Abstraction by the Chlorocarocations: CCl_3^+ and CHCl_2^+ **Jean-Christophe Culmann, Michel Simon, Jean Sommer**
- 1100 A Versatile and Convenient Method for the Preparation of α -(Z)-1-Alkenyl Ketones from β -Keto Benzyl Esters **Shun-ichi Hashimoto, Yoji Miyazaki, Tomohiro Shinoda, Shiro Ikegami**
- 1102 Iron(III) and Copper(II) Catalysed Transformations of Fatty Acid Hydroperoxides: Efficient Generation of Peroxy Radicals with Copper(II) Trifluoromethanesulphonate **Richard K. Haynes, Simone C. Vonwiller**
- 1105 Unexpected Copper(I) Complexation Behaviour observed in the Synthesis of Novel Polynuclear Chromium(0)–Copper(I) Complexes **Raymond Ziessel, Jean Suffert**
- 1107 Substrate Specificity Studies of Aldolase Enzymes for Use in Organic Synthesis **Bruce T. Lotz, Catherine M. Gasparski, Kathleen Peterson, Marvin J. Miller**

- 1110 The Facile Synthesis of a Very Hindered Phenol by Ligand Coupling **Derek H. R. Barton, Dervilla M. X. Donnelly, Patrick J. Guiry, Joseph H. Reibenspies**
- 1111 Stoichiometric Dehydrogenation of Cyclic Alkenes without Hydrogen Acceptors using '(C₅Me₅)Ru⁺' Fragment. X-Ray Crystal Structure of [(η⁵-C₅Me₅)Ru-(μ₂,η⁵,η⁵-C₅Me₄OH)-Ru(η⁵-C₅Me₅)]CF₃SO₃·CH₂Cl₂ **Bruno Chaudret, Françoise Dahan, Xiao Dong He**
- 1113 Structure and Stereochemistry of Pseudolarolide E, a Novel Triterpene Dilactone from *Pseudolarix kaempferi* **Guo-Fu Chen, Zhu-Lian Li, Ke Chen, Cheng-Min Tang, Xiang He, De-Ji Pan, Chang-Qi Hu, Donald R. McPhail, Andrew T. McPhail, Kuo-Hsiung Lee**
- 1115 A Novel Vanadium Pillared Montmorillonite Catalyst for Molecular Recognition of Benzyl Alcohols **B. M. Choudary, V. L. K. Valli**
- 1116 Unusual Kinetically Stable Dialkyltin(IV) Oxides; X-Ray Structures of [(SnR₂(μ-O))₂] and [(SnR₂(OH))₂(μ-O)] [R = CH(SiMe₃)₂] **Michael A. Edelman, Peter B. Hitchcock, Michael F. Lappert**
- 1118 Polynuclear Pentamethylcyclopentadienyl Chloro, Oxo, and Hydroxo Zirconium(IV) Complexes; X-Ray structure of [(η⁵-C₅Me₅)ZrCl₃(μ-Cl)₄(μ₃-O)] and [(η⁵-C₅Me₅)ZrCl(H₂O)(μ-OH)]₂ **Gerardo Hidalgo, Maria Angela Pellinghelli, Pascual Rojo, Ricardo Serrano, Antonio Tiripicchio**
- 1120 Chemoenzymatic Synthesis of (–)-Carbovir utilizing a Whole Cell catalysed Resolution of 2-Azabicyclo[2.2.1]hept-5-ene-3-one **Steven J. C. Taylor, Alan G. Sutherland, Carol Lee, Richard Wisdom, Steve Thomas, Stanley M. Roberts, Christopher Evans**
- 1121 A New Method for the Enantiomeric Excess Determination of Chiral Trisubstituted Allenes by ¹⁹⁵Pt NMR of *trans*-Dichloro[(*S*)-α-methylbenzylamine](allene)platinum(II) Complexes **Piero Salvadori, Gloria Uccello-Barretta, Raffaello Lazzaroni, Anna Maria Caporusso**
- 1123 Biosynthesis of Vitamin B₁₂: Formation of Pyrrocorphins by Peripheral C-Methylation of Precorrin-3 Octamethyl Ester **Colin L. Gibson, Francis Blanche, Alan R. Battersby**
- 1125 Biosynthesis of Vitamin B₁₂: Incorporation of (1*S*)-[11-²H₁]-, and (1*R*)-[11-²H₁]Porphobilinogen into Sirohydrochlorin and 2,7,20-Trimethylisobacteriochlorin **George W. Weaver, Francis Blanche, Denis Thibaut, Laurent Debussche, Finian J. Leeper, Alan R. Battersby**
- 1127 A Synthesis of Novel Perfluorodienes **Mark W. Briscoe, Richard D. Chambers, Steven J. Mullins, Takayuki Nakamura, Frederick G. Drakesmith**
- 1128 A Direct Route to Fluorinated Cyclopentadienes and Cyclopentadienyl Anions **Richard D. Chambers, Martin P. Greenhall**
- 1129 Ruthenium–Arene Complexes and Clusters *via* Ultrasound **Richard S. Bates, Anthony H. Wright**
- 1131 Dramatic Enhancement of the Photoactivity of Zinc Porphyrin–Ellipticine Conjugates by DNA **Steven J. Milder, Li Ding, Guita Etemad-Moghadam, Bernard Meunier, Nicole Paillous**
- 1133 Catalysis Phenomena and Intermediates in the Reaction of Phosphorus Trichloride with Aldehydes **Mukattis B. Gazizov, Rafail A. Khairullin, Roza F. Kadirova, Edward S. Lewis, Alan M. Kook**
- 1135 Modification of Glucose Oxidase by Tetrathiafulvalene **P. N. Bartlett, V. Q. Bradford**

AUTHOR INDEX

- Atkinson, Joseph G., 1072
 Banerji, Ankur A., 1091
 Bartlett, P. N., 1135
 Barton, Derek H. R., 1110
 Bates, Richard S., 1129
 Battersby, Alan R., 1123, 1125
 Beckwith, Athelstan L. J., 1087
 Ben-David, Y., 1090
 Bernstein, Michael A., 1072
 Bevinakatti, Hanamantha S., 1091
 Blanche, Francis, 1123, 1125
 Bradford, V. Q., 1135
 Briscoe, Mark W., 1127
 Caporusso, Anna Maria, 1121
 Chai, Christina L. L., 1087
 Chambers, Richard D., 1127, 1128
 Chaudret, Bruno, 1111
 Chen, Guo-Fu, 1113
 Chen, Ke, 1113
 Chiesi-Villa, Angiola, 1083
 Choudary, B. M., 1115
 Corazza, Fabio, 1083
 Culmann, Jean-Christophe, 1098
 Dahan, Françoise, 1111
 Debussche, Laurent, 1125
 Dickinson, Julia M., 1069
 Ding, Li, 1131
 Donnelly, Dervilla M. X., 1110
 Drakesmith, Frederick G., 1127
 Edelman, Michael A., 1116
 Engel, Robert, 1084
 Etamad-Moghadam, Guita, 1131
 Evans, Christopher, 1120
 Floriani, Carlo, 1083
 Fryzuk, Michael D., 1088
 Fukaya, Toshio, 1096
 Gasparski, Catherine M., 1107
 Gazizov, Mukattis B., 1133
 Gibson, Colin L., 1123
 Girard, Yves, 1072
 Goldberg, Yuri, 1079
 Goodman, Chris, 1069
 Greenhall, Martin P., 1128
 Guastini, Carlo, 1083
 Guiry, Patrick J., 1110
 Haddad, T. S., 1088
 Hamel, Pierre, 1072
 Hashimoto, Shun-ichi, 1100
 Havinga, E. E., 1093
 Haynes, Richard K., 1102
 He, Xiang, 1113
 He, Xiao Dong, 1111
 Hidalgo, Gerardo, 1118
 Hill, Lawrence, 1085
 Hitchcock, Peter B., 1116
 Hu, Chang-Qi, 1113
 Ikegami, Shiro, 1100
 Iovel, Irina, 1079
 Kadirova, Roza F., 1133
 Khairullin, Rafail A., 1133
 Kodaka, Masato, 1096
 Kook, Alan M., 1133
 Lappert, Michael F., 1116
 Lazzaroni, Raffaello, 1121
 Lee, Carol, 1120
 Lee, Kuo-Hsiung, 1113
 Leeper, Finian J., 1125
 Lewis, Edward S., 1133
 Li, Zhu-Lian, 1113
 Lindqvist, Fritiof, 1080
 Lotz, Bruce T., 1107
 McPhail, Andrew T., 1113
 McPhail, Donald R., 1113
 Magnusson, Göran, 1080
 Meijer, E. W., 1093
 Meunier, Bernard, 1131
 Milder, Steven J., 1131
 Miller, Marvin J., 1107
 Milstein, D., 1090
 Misono, Makoto, 1094
 Miyazaki, Yoji, 1100
 Mizuno, Noritaka, 1094
 Mullins, Steven J., 1127
 Murphy, John A., 1069
 Nakamura, Takayuki, 1127
 Newadkar, Ravindra V., 1091
 Nijhuis, S., 1093
 Ohto, Masaru, 1074, 1076
 Orito, Kazuhiko, 1074, 1076
 Paillous, Nicole, 1131
 Pan, De-Ji, 1113
 Patchornik, A., 1090
 Pellinghelli, Maria Angela, 1118
 Peterson, Kathleen, 1107
 Reibenspies, Joseph H., 1110
 Rengan, Kasthuri, 1084
 Reymond, Jean-Louis, 1070
 Richards, Christopher J., 1085
 Rikken, G. L. J. A., 1093
 Rillema, D. Paul, 1081
 Roberts, Stanley M., 1120
 Royo, Pascual, 1118
 Salvadori, Piero, 1121
 Serrano, Ricardo, 1118
 Sherburn, Michael S., 1069
 Shibuya, Isao, 1096
 Shinoda, Tomohiro, 1100
 Shymanska, Mariya, 1079
 Simon, Michel, 1098
 Sommer, Jean, 1098
 Suffert, Jean, 1105
 Suginome, Hiroshi, 1074, 1076
 Sutherland, Alan G., 1120
 Tang, Cheng-Min, 1113
 Taylor, Steven J. C., 1120
 ten Hoeve, W., 1093
 Thibaut, Denis, 1125
 Thomas, Steve, 1120
 Thomas, Susan E., 1085
 Tiripicchio, Antonio, 1118
 Uccello-Barretta, Gloria, 1121
 Valli, V. L. K., 1115
 Van Wallendael, Shawn, 1081
 Vogel, Pierre, 1070
 Vonwiller, Simone C., 1102
 Weaver, George W., 1125
 Wisdom, Richard, 1120
 Wright, Anthony H., 1129
 Wynberg, H., 1093
 Yasuda, Hiroyuki, 1094
 Yonemoto, Katsumi, 1096
 Ziessel, Raymond, 1105

Submission of Journal Manuscripts on Floppy Disks

Summary

There have been various requests by authors to submit manuscripts on floppy disks to a journal for publication. This note details some of the investigations that the RSC has carried out on this subject, some of the problems identified, and some future actions.

Introduction

Many authors who use word processors to prepare papers for submission to RSC journals consider that the information on floppy disk should be readily usable for the production of journals. The potential benefits perceived by the author include reduced proof-reading requirements, reduced costs, and faster publication. At present, however, from the editorial viewpoint, the use of author disks is fraught with many difficulties. There is a need to overcome many technical and organisational problems before the information on floppy disks could be used routinely and efficiently in the production of journals.

The Problems

If the information is to be used for typesetting, the RSC needs to be able to translate word processor formatted documents into the corresponding format with the correct style for the particular journal with footnotes, chemical formulae, diagrams and other figures inserted at the appropriate places for the typesetter.

In 1989 the RSC surveyed about 1000 authors concerning submission of papers on floppy disks to help in assessing the feasibility of accepting such data. About 500 replies were received. The major results were:

- 85% used PCs and associated word-processing software for the preparation of papers submitted to RSC journals.
- 61% of respondents would be willing to submit papers on floppy disk and 45% would be willing to use electronic mail.
- 49% of respondents would be willing to modify their style of writing of papers to conform to RSC requirements of layout or representation of special characters.
- Three main types of computer were used by respondents, IBM PCs and compatibles (43%), Apple Macintoshes (26%) and NEC 9800 series (15% overall, 73% of Japanese respondents).
- Over twenty different word processor software packages were mentioned by two or more authors.
- 67% of Macintosh owners use ChemDraw for chemical structure input.
- There were concerns that electronic submission might become the only form of submission in the future.

From these results it is apparent that the RSC would need to be able to accept information from a wide range of word processors running on a variety of different computers if it was to be able to take papers from all authors in their native format. The RSC would then need to convert these papers to a standard format for editorial work and typesetting without loss of information.

Word processors are becoming more sophisticated. They allow much more tailoring by the end user of various options that can have an effect on the stored document, *e.g.*, different typefaces that have different character sets, complicated formatting options. Different national versions can result in the same computer code being used to represent different characters. At the same time, many word processors have only restricted character set capabilities when compared with the typesetting systems used for setting journals. Authors are often unable to obtain the full range of characters needed for

their papers and use alternatives to obtain a desired visual result (or even write the characters in on the printed manuscript!). Authors also use incorrect characters [*e.g.*, superscript letter o (°) for the degree symbol (°), hyphens for hyphen (-), minus sign (−), en rule (–) and em rule (—) characters]. The presentation of tabular matter, and mathematics causes many difficulties in terms of both the character set and layout.

When authors write papers, they normally lay out the text and other matter in a format that gives the required visual effect and is easy to read when printed on their printer. This may result in the addition of extra hyphens used as end-of-line breaks within text which are not required in the final output.

Unfortunately, the requirements of the RSC are different if it is going to use the information for typesetting. The layout coding used by the authors is normally not readily usable by the RSC (this is particularly true for tabular matter and mathematics). The RSC requirements are likely to include the need for identifiers explicitly marking various sections of text (*e.g.*, title, authors, addresses, footnotes). Formatting to give a visually attractive appearance is not required.

The RSC handles several thousand manuscripts each year. If it is to be able to handle floppy disks of data efficiently then the disks would need to have uniformity of style and content. This would allow each disk to be handled in a standard manner rather than each as an individual item with its own requirements. Ideally the data would be presented in a standard codified format that would allow various items and sections of information to be readily identifiable.

Most chemical papers contain graphical matter, *e.g.*, chemical structures, diagrams, halftones, colour plates. Ideally, these also need to be provided in an acceptable machine-readable format or mechanisms need to be set up to allow their integration into documents.

A Possible Route to Accepting Floppy Disk Information

It should be possible to overcome most, if not all, of these problems in the long term. The implementation of all the necessary systems is unlikely to occur quickly but various steps will be taken in order to move forward. In the short term there is a need to gain more practical experience of problems and solutions by building up case histories.

The RSC survey indicated that a few, widely used word processor formats (*e.g.*, MacWrite, Microsoft Word, WordPerfect, WordStar) are used by a high percentage of authors. There are a few common standards in existence for file interchange (*e.g.*, IBM DCA, Microsoft RTF) to get data into a uniform format for further processing. Other word processors have facilities to convert into these formats or into ASCII format which could be accepted by the RSC. Detailed guidelines are being formulated to assist authors in preparing papers in a codified style and to help the editorial processing of the information.

These guidelines will be used in an experiment, with an invited group of authors in the first instance, to help identify the problems and solutions at a more detailed level.

For further information contact:

Alan McNaught
Manager, Journals
The Royal Society of Chemistry
Thomas Graham House
Science Park, Milton Road
CAMBRIDGE CB4 4WF, UK

Tel: 0223 420066

Fax: 0223 423623

E-mail(JANET): RSC1 @ UK.AC.RL.GB