

X-Ray crystal structure of a new Pb^{II}-selective carbon-pivot lariat ether

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New C-pivot lariat 16-crown-5 ethers and two metal-crown ether complexes are synthesized and characterised by single-crystal X-ray diffraction which indicates that both the crown ring and the side arm are involved cooperatively with the cation (Na⁺ or Pb²⁺) in three-dimensional complexation.

Lariat crown ethers, through the cooperation of crown ring and side arm, often exhibit different cation-binding properties compared with the parent crown ethers.¹ No report concerning the X-ray single-crystal structure of a carbon-pivot lariat crown ether-metal complex has appeared in the literature. We now report our results of two X-ray single-crystal structures of carbon-pivot lariat ether-metal complexes and complexation studies in the gas phase by FAB mass spectroscopy. FABMS has been recognized as a rapid means to characterize metal-ion complexation between crown ethers²⁻⁴ and lariat crown ethers.^{5,6} Since desorption of the substrate from a matrix solution occurs in FAB ionization, a direct observation of the integrity of the complexes in the gas phase is possible. The basic *sym*-dibenzo-16-crown-5 system is chosen for the three-carbon connection with a central hydroxy group providing a handle for easy side-arm attachments, and avoiding the instability of acetal linkage of an all-ethyleneoxy macrocycle.¹ Conventional ion-extraction and transport studies of alkali metals using the parent ring and some lariat crown ethers have been performed.⁷⁻⁹ These methods are tedious and results varied.¹ Furthermore, single-crystal X-ray structures provide concrete evidence for the three-dimensional complexation feature of the side-arm involvement.

Hydroxy-*sym*-dibenzo-16-crown-5 ether **1** was synthesized by modifying the procedures of Cram¹⁰ and coworkers and Bartsch¹¹ and coworkers. 2'-Methoxyethyl-*sym*-dibenzo-16-crown-5 ether **2** was prepared by stirring NaH (0.18 g, 6 mmol) and **1** (1.00 g, 2.89 mmol) in anhydrous thf (30 ml) at 20 °C for 0.5 h under nitrogen; 2-chloroethyl methyl ether (0.293 g, 3.1 mmol) in thf (5 ml) was then added dropwise. After heating the mixture under reflux for 2 h, and destroying the excess NaH with water, thf was removed *in vacuo*. CHCl₃ (50 ml) was added to the residue and extracted with water (2 × 20 ml). After drying (MgSO₄) and passing the CHCl₃ solution through a column of silica gel and eluting with CHCl₃, **2** (0.99 g, 85%), mp 61–62 °C [CHCl₃-hexane (1 : 5)] was obtained.

The complex of **1** (3.46 g, 10 mmol) with NaBr (1.03 g, 10 mmol) was prepared by heating and stirring in ethanol (50 ml, reflux, 72 h). Crystals for X-ray determination were grown by slow evaporation of ethanol. Anal. Calc. (found) for **1**[NaBr]: C, 50.80 (50.66); H, 4.94 (4.89)%. The complex of **2** with Pb(NO₃)₂ was prepared by stirring Pb(NO₃)₂ (0.662 g, 2 mmol) in MeOH-H₂O (4 : 1) (4 ml, *ca.* 25 °C, 5 min) and adding **2** (0.404 g, 1 mmol) in CHCl₃ (1 ml) and stirring for 10 min. X-Ray quality crystals were grown by slow diffusion of hexane into the reaction mixture in a desiccator. Anal. Calc. (found) for **2**[Pb(NO₃)₂]: C, 35.92 (35.89); H, 3.84 (3.77); N, 3.81 (3.83)%. FABMS shows parent-ion peaks with suitable isotopic cluster at *m/z* values for [1 + Na]⁺ and [2 + Pb(NO₃)₂]⁺ both as base peaks (Fig. 1). The crystal structures of **1**[NaBr] and **2**[Pb(NO₃)₂] together with selected bond lengths and angles are shown in Fig. 2.† **1**[NaBr] contains a seven-coordinate pseudo-bipy-

amidal Na ion, with Br⁻ in *cis*-position to the side-arm oxygen [O(1)]. The macroring donor atoms are disposed in a twist-chair conformation with Na⁺ distinctly above the plane of four ring oxygens [O(2), O(3), O(5), O(6)]. The side-arm oxygen is pseudo-axial to the coordination plane. Binding of the side arm can be viewed as occupying one face of the cavity of the macroring donor atoms and cradling the metal ion; thus the cation is immersed deeply in the ring. The lead(II) complex contains eleven-coordinate Pb^{II}, with the macroring donor atoms arranged in a twist-boat structure. The side-arm oxygen occupies a 'flagpole' position cradling the Pb atom toward the crown rings as seen in Fig. 2(b). The lariat's cavity in the complex is more flexible than that of the parent crown ether and can adjust to an optimum size for each cation.

FABMS was used to assess the binding ability between the lariat crown ether and cations in *m*-nitrobenzyl alcohol. In addition to the parent-ion peaks, fragments from the [2 + Pb]⁺ complex were observed as an isotope cluster at *m/z* 509, 611, 612 and 613. Since the parent crown ether **1** is known to show selectivity towards Na,¹² a competitive complexation of equimolar **1** and **2** with Na⁺ was undertaken with adequate calibration¹³ and should give an evaluation of the side-arm effect. Besides strong signals for [2 + Na]⁺ and [1 + Na]⁺ at *m/z* 427 and 369, protonated and molecular ions were observed at *m/z* 405 [2 + H]⁺, 404 [2]⁺ and 347 [1 + H]⁺, 346 [1]⁺, respectively. The ratios of [2 + Na]⁺/[2]⁺ and [1 + Na]⁺/[1]⁺ were *ca.* 12 and 0.15, respectively. Thus the ethylenemethoxy side arm enhances sodium selectivity *ca.* sevenfold. Since no 2 : 1 complex peaks were observed, lariat ethers provide a bound cation with three-dimensional complexation without requiring a sandwich structure.¹⁴ Preferential complexation of **2** with Pb²⁺ among heavy-metal ions (Zn²⁺, Hg²⁺, Pb²⁺, Ag⁺, Cu²⁺) was also

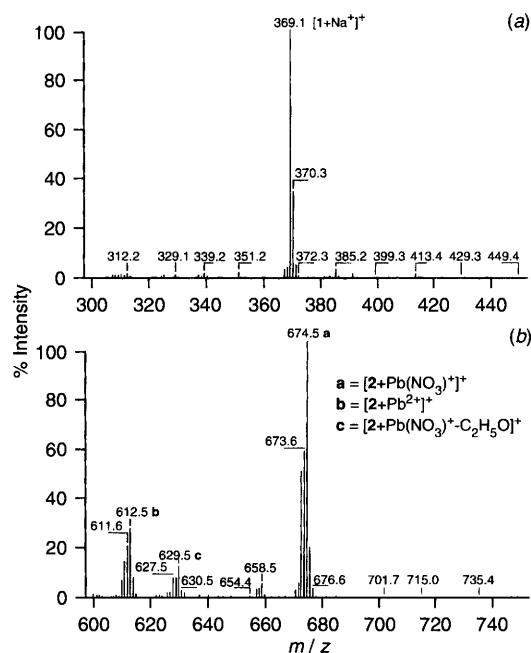


Fig. 1 FAB mass spectrum of (a) [1 + NaBr] and (b) [2 + Pb(NO₃)₂]

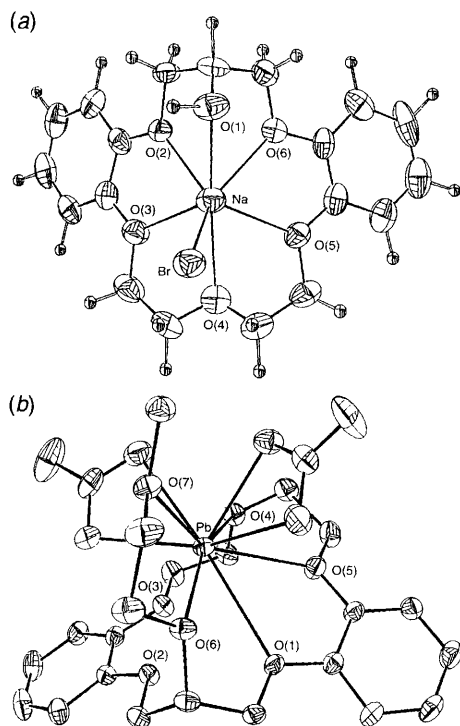


Fig. 2 (a) Structure of **1**[NaBr] with selected bond lengths (Å) and angles (°): Na–O(1) 2.453(5), Na–O(2) 2.425(6), Na–O(3) 2.553(6), Na–O(4) 2.721(6), Na–O(5) 2.530(6), Na–O(6) 2.479(6), Na–Br 2.883(3); Br–Na–O(1) 86.4(1), O(1)–Na–O(2) 69.1(2), O(2)–Na–O(3) 62.0(2), O(3)–Na–O(4) 60.5(2), O(4)–Na–O(5) 60.7(2), O(5)–Na–O(6) 62.0(2). (b) Structure of **2**[Pb(NO₃)₂] with selected bond lengths (Å) and angles (°): Pb–O(1) 2.903(4), Pb–O(4) 2.801(4), Pb–O(5) 2.857(4), Pb–O(6) 2.634(4), Pb–O(7) 2.770(4), Pb–O(10) 2.581(5), Pb–O(11) 2.638(4), Pb–O(13) 2.580(4), Pb–O(14) 2.742(4); O(1)–Pb–O(5) 54.7(1), O(1)–Pb–O(6) 58.9(1), O(4)–Pb–O(5) 57.9(1), O(6)–Pb–O(7) 60.5(1).

indicated by FABMS. No peak corresponding to $[2 + M(\text{anion})_{0-1}]^+$ other than for Pb was observed; and $[2 + \text{Pb}(\text{NO}_3)_2]^+$, m/z 674 was the base peak.

In conclusion, side-arm involvement of lariat ethers in cooperating cation binding is demonstrated by both single-crystal X-ray diffraction and FABMS. Attachment of a side arm enhances binding towards Na⁺ and selectivity towards Pb²⁺. The ease of synthesis and the flexibility of the lariat crown ethers suggest many promising applications for these compounds as complexing agents.

We thank the National Science Council of the Republic of China for financial support (Grant No. NSC 84-2113-M003-004).

Footnote

† *Crystal data:* **1**[NaBr], C₁₉H₂₂BrNaO₆, white crystals, orthorhombic, space group $P2_12_12_1$, $a = 8.660(2)$, $b = 13.121(3)$, $c = 17.246(9)$ Å, $U =$

1960(1) Å³, $Z = 4$, $D_c = 1.523$ Mg m⁻³. Data collection carried out on a Nonius CAD-4 diffractometer using graphite-monochromated Mo-K α radiation at 25 °C. Atomic scattering factors were taken from ref. 15, and data reduction and structural refinement were performed using NRCC-SDP-VAX packages.¹⁶ Absorption corrections were made by the empirical Ψ -rotation method. Cell parameters were obtained from 25 reflections with 2θ 23.14–27.26°. A total of 1984 unique reflections were collected and the data were corrected for decay and absorption.¹⁶ A total of 1551 reflections with $I > 2.5\sigma(I)$ were used in the refinement. The structure was solved by direct methods and refined by least-squares cycles. All the non-H atoms were refined with anisotropic thermal parameters. Full-matrix least-squares refinement led to convergence with $R = 0.040$, $R' = 0.033$.

2[Pb(NO₃)₂], C₂₂H₂₈N₂O₁₃Pb, white crystals, monoclinic, space group $P2_1/n$, $a = 11.031(2)$, $b = 9.187(3)$, $c = 25.426(5)$ Å, $\beta = 96.86(2)^\circ$, $U = 2558(1)$ Å³, $Z = 4$, $D_c = 1.910$ Mg m⁻³. Intensities of 4489 unique reflections in the region $2\theta < 49.8^\circ$. Cell parameters were obtained from 25 reflections with 2θ 23.54–27.18°. A total of 3403 reflections with $I > 2.5\sigma(I)$ were used in the refinement; $R = 0.027$, $R' = 0.021$.

Atomic coordinates, bond lengths and angles, and thermal parameters have been deposited at the Cambridge Crystallographic Data Centre (CCDC). See Information for Authors, Issue No. 1. Any request to the CCDC for this material should quote the full literature citation and the reference number 182/56.

References

- G. W. Gokel, *Chem. Soc. Rev.*, 1992, **21**, 39 and references therein.
- R. A. W. Johnstone and M. E. Rose, *J. Chem. Soc., Chem. Commun.*, 1983, 1268.
- K. Yamada, S. Matsutani, A. Uchiyama and T. Takahashi, *J. Incl. Phenom.*, 1991, **11**, 49.
- M. Sawasda, Y. Okumura, H. Yamada, Y. Takai, S. Takahashi, T. M. Kaneda, K. Hirose and S. Miusmi, *Org. Mass Spectrom.*, 1993, **28**, 1525.
- T. Takahashi, A. Uchiyama, K. Yamada, B. C. Lynn and G. W. Gogel, *Tetrahedron Lett.*, 1992, **33**, 3825.
- Y. Habata, M. Ikeda and S. Akabori, *J. Chem. Soc., Perkin Trans. 1*, 1992, 2651.
- R. A. Bartsch, *Soln. Extn. Ion Exch.*, 1989, **7**, 829.
- C. J. Pedersen, *J. Am. Chem. Soc.*, 1970, **92**, 391.
- W. Walkowiak, W. A. Charewicz, S. I. Kang, I. W. Yang, W. J. Pugia and R. A. Bartsch, *Anal. Chem.*, 1990, **62**, 2018 and references therein.
- E. P. Kyba, R. C. Helgeson, K. Madan, G. W. Gokel, T. L. Arroeski, S. S. Moore and D. J. Cram, *J. Am. Chem. Soc.*, 1977, **99**, 2564.
- G. S. Heo, R. A. Bartsch, L. L. Schlobohm and J. G. Lee, *J. Org. Chem.* 1981, **46**, 3574.
- Z. O. Tuarsheva, Y. G. Mamedova, A. L. Shabanov and G. A. Sidakova, *Zh. Org. Khim.*, 1984, **20**, 404; *Chem. Abstr.*, 100 209777m.
- C. J. Langley, D. G. Hamilton and M. C. Gossel, *J. Chem. Soc., Perkin Trans. 2*, 1995, 929.
- H. Tsukube, J. Uenishi, H. Higaki, K. Kikkawa, T. Tanaka, S. Wakabayashi and S. Oae, *J. Org. Chem.*, 1993, **58**, 4389.
- International Tables for X-ray Crystallography*, Kynoch Press, Birmingham, 1974, vol. 4.
- A. C. Larson, F. L. Lee, P. Y. Le, M. Webster, J. P. Charland and E. J. Gabe NRCVAX Crystal Structure System. Chemistry Division, NRC, Ottawa, Canada, 1990.

Received, 19th February 1996; Com. 6/01167E

Conference Diary*

June 1996

1996 International Conference on Intelligent Materials

Lyon, France June 3-5
Contact: Mrs Claude Bernavon, ICIM 96, Group d'Etudes de Metallurgie Physique et de Physique de Materiaux, Bât. 502 - 1er étage, Institut National des Sciences Appliquées de Lyon, 20 avenue Albert Einstein, F 69621 Villeurbanne Cedex, France.
Tel +33 72 43 83 85. Fax +33 72 43 88 30.
E-mail bernavon@insa.insa-lyon.fr

13th International Summer School on Organometallic Chemistry

Karpacz, Poland June 2-8
Contact: Professor P Sohota or Professor J Ziolkowski, Institute of Chemistry, University of Wrocław, 14 F. Joliot-Curie Street, 50-383 Wrocław, Poland.

26th Reaction Mechanisms Conference

Stony Brook, USA June 7-12
Contact: William le Noble, Department of Chemistry, SUNY at Stony Brook, Stony Brook, NY 11794-3400, USA.
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E-mail wlenoble@sunysb.edu

2nd EUCHEM Conference on Nitrogen Ligands in Organometallic Chemistry and Homogeneous Catalysis

Villa Olmo, Como, Italy June 9-14
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Electronic Materials for Displays

London, UK June 12
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70th Colloid and Surface Science Symposium

Potsdam, USA June 16-19
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International Congress: Progress of the Science and Technology of Gold

Hanau, Germany June 16-20
Contact: Professor H Schmidbaur, Anorganisch-Chemisches Institute, Technische Universität München, Lichtenbergstrasse 4, D 85747 Garching, Germany. Fax +49 (89) 3209 3125.

18th International Conference in Stabilization and Controlled Degradation of Polymers

Luzern, Switzerland June 17-19
Contact: Dr A V Patsis, Director, Institute for Materials Science, State University of New York, New Paltz, NY 12561, USA.
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International Symposium on Theoretical and Experimental Aspects of Protein Folding

San Luis City, Argentina June 17-20
Contact: Dr J Vila, IMASL-Universidad Nacional de San Luis, Ejercito de Los Andes 950, 5700 San Luis, Argentina.

25th National Medicinal Chemistry Symposium

Ann Arbor, MI, USA June 18-22
Contact: L B Townsend, University of Michigan, 428 Church St, 1028 College of Pharmacy, Ann Arbor, MI 48109, USA.
Tel +1 313 764 7547. Fax +1 313 763 2022.

Clean Tech '96

Uxbridge, UK June 19-21
Contact: Conference Secretariat, SCI, 14/15 Belgrave Square, London, UK SW1X 8PS. Fax +44 (0) 171 823 1698.

79th Canadian Society for Chemistry Conference

St. John's, Canada June 23-27
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E-mail CSCXT@ACADVM1.UOTTAWA.CA

XXI International Symposium on Macrocyclic Chemistry

Montecatini Terme, Italy June 23-28
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11th Conference on Polymers. Thermal and Photo-induced Oxidation of Polymers and its Inhibition in the upcoming 21st Century

High Tatras, Slovak Republic June 24-28
Contact: Professor L Rychlá, Polymer Institute, Slovak Academy of Sciences, Dubravská cesta 9, 842 36 Bratislava, Slovak Republic.

16th International Liquid Crystal Conference

Kent, USA June 24-28
Contact: 16th International Liquid Crystal Conference, Liquid Crystal Institute, Kent State University, PO Box 5190, Kent, OH 44242-0001, USA. Tel +1 216 672 2654.
Fax +1 216 672 2796. E-mail ILCC16@alice.kent.edu

EUCHEM Conference on Chemistry and Biology of Carbohydrate Therapeutics

Stockholm, Sweden June 24-28
Contact: The Swedish National Committee for Chemistry, Wallingatan 24 3tr, S-111 24 Stockholm, Sweden.
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11th International Conference on Surface Forces

Moscow, Russia June 25-29
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11th IUPAC International Conference on Organic Synthesis

Amsterdam, The Netherlands June 30-July 4
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Baltimore, USA June 30-July 5
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Yeppoon, Australia June 30-July 5
Contact: Professor R Warrener, 15NOC, C/-Chemistry Department, Central Queensland University, Rockhampton, Qld 4702, Australia. Tel +61 (0) 79 30 9919. Fax +61 (0) 79 30 9917. E-mail 15NOC@cqu.edu.au

July 1996**14th International Conference on Radical Ions**

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Contact: Ms Mari Löfkvist, Secretary Radical Ions 14, Department of Physics, IFM, Linköping University, S-581 83 Linköping, Sweden.

Solid State Chemistry '96

Bratislava, Slovak Republic July 6-12
Contact: SSCH '96, Institute of Inorganic Chemistry, Slovak Academy of Sciences, SK-842 36 Bratislava, Slovak Republic.

Recent Advances in the Chemistry of Anti-infective Agents

Cambridge, UK July 7-10
Contact: Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, UK BS19 2FQ. Tel & Fax +44 (0) 1275 853311.

5th Meeting of the European Society of Sonochemistry

Cambridge, UK July 7-11
Contact: RSC†

XVIIth International Conference, Organometallic Chemistry

Brisbane, Australia July 7-12
Contact: XVIIth ICOMC Secretariat, Faculty of Science and Technology, Griffith University, Brisbane, Qld 4111, Australia. E-mail ICOMC@sct.gu.edu.au

17th International Symposium on the Organic Chemistry of Sulfur

Tsukuba, Japan July 7-12
Contact: Dr Norihiro Tokitoh, Executive Secretary, ISOCS-17, Department of Chemistry, Graduate School of Science, The University of Tokyo, 7-3-1 Hongo, Bunkyo-Ku, Tokyo 113, Japan. Tel & Fax +81 3 5800 6899. E-mail chisocs@chem.s.u-tokyo.ac.jp

Carbon '96

Newcastle upon Tyne, UK July 7-12
Contact: RSC†

World Congress of Theoretical Organic Chemists

Jerusalem, Israel July 7-12
Contact: KENES POB 50006, Tel Aviv 61500, Israel.

6th International Meeting: Reaction Mechanisms

Canterbury, UK July 8-12
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6th Belgian Organic Synthesis Symposium

Gent, Belgium July 8-12
Contact: Professor M Vandewalle, Universiteit Gent, Vakgroep Organische Chemie, Krijgslaan, 281(S4), B-9000 Gent, Belgium. Tel +32 9 264 4460. Fax +32 9 264 49 98.

IX International Meeting on Boron Chemistry

Heidelberg, Germany July 14-18
Contact: Dr M Enders, Ruprecht-Karls, Universität Heidelberg, Anorganisch-Chemisches Institut, Im Neuenheimer Feld 270, D-69120 Heidelberg, Germany.

International Symposium on Sweeteners

Jerusalem, Israel July 14-20
Contact: Sweeteners, PO Box 50006, Tel-Aviv 61500, Israel. Tel +972 3 5140014. Fax +972 35175674/5140077.

RSC 5th International Symposium: Progress in Natural Product Chemistry

Nottingham, UK July 15-18
Contact: RSC†

XVIIIth International Conference on Polyphenols

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Contact: Professor J Vercauteren, Lab. Pharmacognosie, Université Bordeaux 2, 146 rue Léo Saignat, 33076 Bordeaux Cedex, France. Tel +33 57 57 12 60. Fax +33 56 96 09 75. E-mail Joseph.Vercauteren@gnosie.u-bordeaux2.fr

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Milan, Italy July 15-21
Contact: Professor B Casu, G. Ronsoni Inst. for Chemical and Biochemical Research, Via G Colombo 81, 20133 Milan, Italy. Fax +39 270633007.

XVIth IUPAC Symposium on Photochemistry

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6th International Conference on the Chemistry of the Platinum Group Metals

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International Conference on Science and Technology of Synthetic Materials

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10th American Conference on Crystal Growth

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10th International Symposium on Homogeneous Catalysis

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31st International Conference on Coordination Chemistry

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Contact: Professor C Orvig, Department of Chemistry, University of British Columbia, Vancouver, BC, Canada V6T 1Z1. Tel +1 604 822 4449. Fax +1 604 822 2847. E-mail orvig@chem.ubc.ca

International Symposium on Macromolecular Condensed State

Beijing, China August 20-25
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Leuven, Belgium August 28-31
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Supramolecular Chemistry: Molecular Recognition and Drug-Receptor Interactions

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Contact: Dr J Hendekovic, European Science Foundation, 1 quai Lezay-Marnésia, 67080 Strasbourg Cedex, France. Tel +33 88 76 71 35. Fax +33 88 36 69 87. E-mail euresco@esf.org

September 1996

NSW Southern Highlands Conference on Heterocyclic Chemistry

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Contact: Professor David St C Black, School of Chemistry, University of New South Wales, Sydney, NSW 2052, Australia. Tel +61 2 385 4712. Fax +61 2 662 2835. E-mail D.Black@unsw.edu.au

8th FECEM Conference on Heterocycles in Bio-organic Chemistry

Villa Olmo, Como, Italy September 1-4
Contact: Professor Bruno Danieli, Dipartimento di Chimica Organica e Industriale, Università di Milano, Via Golgi 19, I-20133 Milano, Italy.

ECME 96, Third European Conference on Molecular Electronics

Leuven, Belgium September 1-6
Contact: Professor F C De Schryver, Department of Chemistry, KU. Leuven, Celestijnenlaan 200 F, B-3001 Heverlee, Belgium.

XIth International Symposium on Organosilicon Chemistry

Montpellier, France September 1-6
Contact: Professor R J P Corriu, Laboratoire des Précurseurs Organométalliques de Matériaux, UMR CNRS 44, Université de Montpellier II, Place E. Bataillon, CC 007, F34095 Montpellier Cedex 5, France. Fax +33 67 14 38 88.

11th European Symposium on Quantitative Structure-Activity Relationships: Computer-assisted Lead Finding and Optimization

Lausanne, Switzerland September 1-6
Contact: Dr Han van de Waterbeemd, c/o F. Hoffmann-La Roche Ltd, Dept. PRPC 65/314, CH-4002 Basel, Switzerland. Tel +41 61 688 8421. Fax +41 61 688 1075. E-mail johannes.van_de_waterbeemd@roche.com

5th International Conference on Chemical Synthesis of Antibiotics and Related Microbial Products

Debrecen, Hungary September 1-6
Contact: The Congress Center, L. Kossuth University, 5th ICSA, H-4010 Debrecen, PO Box 68, Hungary. Fax +36 52 310936. E-mail antibiotics@tigris.klte.hu

RSC 3rd International Symposium: Transition Metals in Organic Synthesis

London, UK September 4-6
Contact: RSC†

Biocoordination Chemistry and Framework Structures

Odense, Denmark September 6-11
Contact: Professor H Toftlund, Kenusk Institut, Department of Chemistry, Odense Universitet, Campusvej 55, DK-5230 Odense M, Denmark.

9th International Symposium on Molecular Recognition and Inclusion (ISMRI9)

Lyon, France September 7-12
Contact: Dr A W Coleman, Institute de Chimie et Biologie des Protéines, CNRS UPR 417, 7 Passage du Vercors, F-69376 Lyon Cedex 07, France. Tel +33 72 72 26 40. Fax +33 72 72 26 01.

†*Contact:* Dr J F Gibson, The Royal Society of Chemistry, Burlington House, London, UK W1V 0BN. Tel +44 (0) 171 437 8656. Fax +44 (0) 171 734 1227. E-mail Conferences@rsc.org

XIVth International Symposium on Medicinal Chemistry
Maastricht, The Netherlands September 8-12
Contact: H Timmerman, Leiden/Amsterdam Centre for Drug Research (LACDR), Department of Pharmacochimistry, Vrije University, De Boelelaan 1083, NL-1081-HV Amsterdam, The Netherlands. Tel +31 (0) 20 44 47580. Fax +31 (0) 20 44 47610. E-mail bijloo@chem.vu.nl

4th International Symposium on Heterogeneous Catalysis and Fine Chemicals
Basel, Switzerland September 8-12
Contact: 4th International Symposium on HCFC '96, c/o AKM Congress Service, PO Box, CH-4005 Basel, Switzerland. Tel +41 61 691 51 11. Fax +41 61 691 81 89.

XIIIth International Symposium on the Reactivity of Solids
Hamburg, Germany September 8-12
Contact: Secretary XIIIth ISRS, Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany. Tel +49 40 41 23 60 86. Fax +49 40 41 23 63 48.

RSC 24th Symposium of the European Peptide Society
Edinburgh, UK September 8-13
Contact: RSC†

Molecular Modelling of Chemicals and Materials
Amsterdam, The Netherlands September 9-10
Contact: Dr A M Brouwer, Laboratory of Organic Chemistry, Amsterdam Institute of Molecular Studies (AIMS), Nieuwe Achtergracht 129, 1018 WS Amsterdam, The Netherlands. Fax +31 (0) 20 5255670. E-mail mgms@chem.uva.nl WWW <http://krop.chem.uva.nl/mgms/>

Advances in Chemistry of Crop Protection
Cambridge, UK September 9-11
Contact: Conference Secretariat, SCI, 14/15 Belgrave Square, London, UK SW1X 8PS. Tel +44 (0) 171 235 3681. Fax +44 (0) 171 823 1698.

14th International Symposium on Gas Kinetics
Leeds, UK September 9-12
Contact: RSC†

RSC Autumn Meeting
Uxbridge, UK September 10-13
Contact: RSC†

Reactivity in Organised Microstructures: Chemical Reactions and Physical Processes in Compartmentalized Systems
Santiago de Compostela, Spain September 10-15
Contact: Dr J Hendeckovic, European Science Foundation, 1 quai Lezay-Mamésia, 67080 Strasbourg Cedex, France. Tel +33 88 76 71 35. Fax +33 88 36 69 87. E-mail euresco@esf.org WWW <http://www.esf.org/euresco>

COPS-IV 4th International Symposium on the Characterisation of Porous Solids
Bath, UK September 15-18
Contact: Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, UK BS19 2FQ. Tel & Fax +44 (0) 1275 853311.

20th IUPAC Symposium on the Chemistry of Natural Products
Chicago, USA September 15-20
Contact: IUPAC Symposium Headquarters, 5999 Butterfield Road, Hillside, IL 60162, USA. E-mail IUPAC@searle.monsanto.com www <http://www.a2z.com/iupac20/index.html>

Faraday Discussion 104, Complex Fluids and Interfaces
Cambridge, UK September 18-20
Contact: RSC†

3rd International Medicinal Chemistry Symposium
Bath, UK September 22-24
Contact: Elaine Wellingham, Conference Secretariat, Field End House, Nailsea, Bristol, UK BS19 2FQ. Tel & Fax +44 (0) 1275 853311. E-mail i.s.blagbrough@bath.ac.uk and m.d.threadgill@bath.ac.uk

23rd Annual Conference of the Federation of Analytical Chemistry and Spectroscopic Societies, FACSS XXIII
Kansas City, USA September 29-October 4
Contact: FACSS National Office, 201-B Broadway St., Frederick, MD 21701-6501 USA. Tel +1 301 846 4797. Fax +1 301 694 6860.

October 1996

XVIIth European Colloquium of Heterocyclic Chemistry
Regensburg, Germany October 6-9
Contact: Professor G Märkl, Institut für Organische Chemie, Universität Regensburg, D-93040 Regensburg, Germany. Tel +49 941 943 4631. Fax +49 941 943 4505.

Joint RSC Fine Chemicals and Medicinals Group-SCI Cardiovascular Meeting
Edinburgh, UK October 20-22
Contact: RSC†

Recent Advances in Drugs for the Treatment of Cardiovascular Disease
Edinburgh, UK October 20-22
Contact: Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, UK BS19 2FQ. Tel & Fax +44 (0) 1275 853311.

December 1996

Fifth Eurasia Conference on Chemical Sciences
Guangzhou, China December 10-14
Contact: Professor Liang-Nian Ji, Biotechnology Research Center, Zhongshan (Sun Yatsen) University, Guangzhou, Canton 510275, China. Tel +86 (20) 418 5461. Fax +86 (20) 418 9173. E-mail leiy@bepc2.ihep.ac.cn

Faraday Discussion 105, Catalysis and Surface Science at High Resolution
Reading, UK December 16-18
Contact: Professor M Bowker, Department of Chemistry, University of Reading, Whiteknights Park, Reading, UK RG6 6AD.

January 1997

International Symposium on Chemical and Biological Thermodynamics
Amritsar, India January 5-8
Contact: Professor D V S Jain, Department of Chemistry, Panjab University, Chandigarh 160014, India. Tel +91 (172) 541435. Fax +91 (172) 541409. E-mail dvs-jain@imtech.ernet.in

April 1997

Spring ACS National Meeting
San Francisco, USA April 13-17
Contact: American Chemical Society, Meetings, PO Box 18598, 20th St Station, Washington, DC 20036-8598, USA.

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