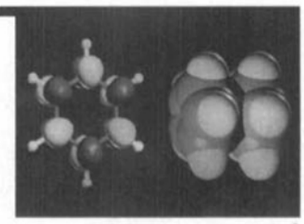
(0,095 mol) gepulvertem NaOH und 5,8 ml (0,2 mol) frisch destilliertem CH_3I versetzt. Die Mischung wird bei RT. 2 h gerührt, mit 30 ml AcOEt verdünnt und anschliessend 5 x mit H_2O gewaschen. Die org. Phase wird getrocknet und i.V. eingeengt. Das zurückbleibende Öl wird mit wenig Et_2O versetzt und zur Kristallisation gebracht. Nach Reinigung der Kristalle über Kieselgel (Kieselgel *60*, Korngrösse 0,04–0,063 mm, Laufmittel: AcOEt/Hexan 94:6) werden 0,920 g eines Gemisches hochmethylierter β-Cyclodextrine mit einem Schmelzbereich von 86–95° erhalten.

Eingegangen am 21. Dezember 1990

[1] T. Tanaka, S. Kurozumi, T. Toru, S. Miura, M. Kobayashi, S. Ishimoto, *Tetrahedron* **1976**, *32*, 1713.
[2] S. Takano, K. Tanigawa, K. Ogasawara, *J. Chem. Soc. ,Chem. Commun.* **1976**, 189.
[3] M. Nara, S. Terashima, S. Yamada, *Tetrahedron* **1980**, *36*, 3161.
[4] R. Noyori, M. Suzuki, *Angew. Chem.* **1984**, *96*, 854.
[5] M. Harre, P. Raddatzt, R. Walenta, E. Winterfeld, *Angew. Chem.* **1982**, *94*, 496.
[6] S. Miura, S. Kurozumi, T. Toru, M. Kobayashi, S. Matsubara, S. Ishimoto, *Tetrahedron* **1976**, *32*, 1893.
[7] K. Laumen, M. Schneider, *Tetrahedron Lett.* **1984**, *25*, 5875.
[8] K. Laumen, E. H. Reimerdes, M. Schneider, H. Görisch, *Tetrahedron Lett.* **1985**, *26*, 407.
[9] Y.-I. Wang, C.-S. Chen, G. Girdaukas, C. J. Sih, *J. Am. Chem. Soc.* **1984**, *106*, 3695.
[10] T. Sugai, K. Mori, *Synthesis* **1988**, 18.
[11] D. R. Deardorff, A. J. Matthews, D. S. McMeekin, C. L. Craney, *Tetrahedron Lett.* **1985**, *26*, 5615; *ibid.* **1986**, *26*, 1255.
[12] K. Laumen, M. Schneider, *J. Chem. Soc., Chem. Commun.* **1986**, 1298.
[13] F. Theil, S. Ballschuh, H. Schick, M. Haupt, B. Häfner, S. Schwarz, *Synthesis* **1988**, 540.
[14] P. J. Keller, E. Cohen, H. Neurath, *J. Biol. Chem.* **1958**, *233*, 344.
[15] G. Marchis-Mouren, M. J. Constantin, P. Desnuelle, *Bull. Soc. Chim. Biol.* **1958**, *40*, 2019.
[16] G. Alexander, Z. Jurvancz, J. Szejtli, *J. High Res. Chrom. Chrom. Commun.* **1988**, 11, 110.
[17] V. Schurig, H. P. Novotny, *J. Chromatogr.* **1988**, *441*, 155.
[18] W. A. König, *Nachr. Chem. Tech. Lab.* **1989**, *37*, 471.
[19] D. W. Armstrong, W. Li, C. D. Chang, J. Pitha, *Anal. Chem.* **1990**, *62*, 914.
[20] Z. Jurvancz, G. Alexander, J. Szejtli, *J. High Res. Chrom. Chrom. Commun.* **1987**, *10*, 105.
[21] H. P. Novotny, D. Schmalring, D. Wistuba, V. Schurig, *J. High Res. Chrom. Chrom. Commun.* **1989**, *12*, 383.
[22] J. Mraz, L. Feltl, E. Smolkowa-Keulemansova, *J. Chromatogr.* **1984**, *286*, 17.
[23] G. Fabian, A. Knoll, F. Theil, M. Böhme, in Vorbereitung.
[24] K. Grob, 'Making and Manipulating Capillary Collumns for Gas Chromatography', Dr. Hüthig Verlag, München, 1986, S. 156 ff.
[25] F. Theil, H. Schick, M. A. Lapitzkaya, K. K. Pivnitzky, *Liebigs Ann. Chem.*, im Druck.
[26] P. A. Grieco, *J. Org. Chem.* **1972**, *37*, 2363.

COMPUTATIONAL CHEMISTRY COLUMN

Column Editors:
Prof. Dr. J. Weber, University of Geneva
PD Dr. H. Huber, University of Basel
Dr. H. P. Weber, Sandoz AG, Basel



Editors' Note

We would like to remind our readers that their contributions to this *Column* are most welcome, in the form of comments, letters, *etc.*, relating to any topic of general interest in computational chemistry or to the subjects presented in previous issues. It is indeed one of the main purposes of the *Column* to be a forum where, in addition to the publication of general articles, ideas could be exchanged and, would it be the case, debated for the sake of providing new information to our readership.

Chimia 45 (1991) 198–199

Computational Chemistry in Switzerland and the Future HLR-91 Supercomputer

All Swiss scientists, and chemists are no exception, specialized in supercomputing are aware of the developments of the HLR-91 (HLR = Hochleistungsrechner) project. However, in view of its importance and the new possibilities it offers to Swiss computational chemists, we found it worthwhile to present and discuss the HLR-91 project in some detail in this Column, keeping in mind that most of our readers are probably not specialized in (super)computers.

All the story started a few years ago when the Swiss federal parliament voted a budget of 40 Mio SFr. for encouraging and developing the use of supercomputers by the universities and federal institutes of technology of our country. This gave birth to the so-called HLR-91 project consisting essentially in the acquisition of a third HLR in Switzerland (in addition to the CRAY-YMP and CRAY-2 machines installed at ETHZ and EPFL, respectively) and to have it functioning in the early nineties. There is no doubt that this project is both important and timely, as high-level research in several fields can no longer be achieved without resorting to large-scale calculations on supercomputers with performance rates of the order of 100–1000 Mflops (1 Mflop = 1 million floating point operations per second). It is indeed a truism to state that supercomputers have become indispensable in the following applications (the list being not exhaustive):

- computational fluid dynamics (*e.g.* turbulence and combustion processes)
- structural analysis (*e.g.* crash simulation)
- wheather forecasting and climate research
- quantum chemistry and macromolecular modelling (*e.g.* drug design and protein folding)
- materials science (*e.g.* new high-T_c super-conductors)
- plasma physics
- seismic explorations.

There was, therefore, every reason to believe that the research projects undertaken in these fields and in progress in Swiss universities and ETHs would also take advantage of supercomputing facilities, and the Swiss parliament and high authorities should be thanked for having initiated the HLR-91 project. So, today, five years after the installation of the first supercomputer in Switzerland (CRAY-1S at EPFL), where are we going with HLR-91?

After many years of long discussions within several *ad-hoc* committees (under our latitudes, the decisional procedures are always slower than one would normally expect), the final decisions concerning HLR-

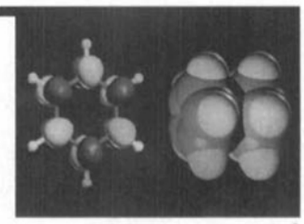
(0,095 mol) gepulvertem NaOH und 5,8 ml (0,2 mol) frisch destilliertem CH_3I versetzt. Die Mischung wird bei RT. 2 h gerührt, mit 30 ml AcOEt verdünnt und anschliessend 5 x mit H_2O gewaschen. Die org. Phase wird getrocknet und i.V. eingeengt. Das zurückbleibende Öl wird mit wenig Et_2O versetzt und zur Kristallisation gebracht. Nach Reinigung der Kristalle über Kieselgel (Kieselgel *60*, Korngrösse 0,04–0,063 mm, Laufmittel: AcOEt/Hexan 94:6) werden 0,920 g eines Gemisches hochmethylierter β-Cyclodextrine mit einem Schmelzbereich von 86–95° erhalten.

Eingegangen am 21. Dezember 1990

[1] T. Tanaka, S. Kurozumi, T. Toru, S. Miura, M. Kobayashi, S. Ishimoto, *Tetrahedron* **1976**, *32*, 1713.
[2] S. Takano, K. Tanigawa, K. Ogasawara, *J. Chem. Soc. ,Chem. Commun.* **1976**, 189.
[3] M. Nara, S. Terashima, S. Yamada, *Tetrahedron* **1980**, *36*, 3161.
[4] R. Noyori, M. Suzuki, *Angew. Chem.* **1984**, *96*, 854.
[5] M. Harre, P. Raddatzt, R. Walenta, E. Winterfeld, *Angew. Chem.* **1982**, *94*, 496.
[6] S. Miura, S. Kurozumi, T. Toru, M. Kobayashi, S. Matsubara, S. Ishimoto, *Tetrahedron* **1976**, *32*, 1893.
[7] K. Laumen, M. Schneider, *Tetrahedron Lett.* **1984**, *25*, 5875.
[8] K. Laumen, E. H. Reimerdes, M. Schneider, H. Görisch, *Tetrahedron Lett.* **1985**, *26*, 407.
[9] Y.-I. Wang, C.-S. Chen, G. Girdaukas, C. J. Sih, *J. Am. Chem. Soc.* **1984**, *106*, 3695.
[10] T. Sugai, K. Mori, *Synthesis* **1988**, 18.
[11] D. R. Deardorff, A. J. Matthews, D. S. McMeekin, C. L. Craney, *Tetrahedron Lett.* **1985**, *26*, 5615; *ibid.* **1986**, *26*, 1255.
[12] K. Laumen, M. Schneider, *J. Chem. Soc., Chem. Commun.* **1986**, 1298.
[13] F. Theil, S. Ballschuh, H. Schick, M. Haupt, B. Häfner, S. Schwarz, *Synthesis* **1988**, 540.
[14] P. J. Keller, E. Cohen, H. Neurath, *J. Biol. Chem.* **1958**, *233*, 344.
[15] G. Marchis-Mouren, M. J. Constantin, P. Desnuelle, *Bull. Soc. Chim. Biol.* **1958**, *40*, 2019.
[16] G. Alexander, Z. Jurvancz, J. Szejtli, *J. High Res. Chrom. Chrom. Commun.* **1988**, 11, 110.
[17] V. Schurig, H. P. Novotny, *J. Chromatogr.* **1988**, *441*, 155.
[18] W. A. König, *Nachr. Chem. Tech. Lab.* **1989**, *37*, 471.
[19] D. W. Armstrong, W. Li, C. D. Chang, J. Pitha, *Anal. Chem.* **1990**, *62*, 914.
[20] Z. Jurvancz, G. Alexander, J. Szejtli, *J. High Res. Chrom. Chrom. Commun.* **1987**, *10*, 105.
[21] H. P. Novotny, D. Schmalring, D. Wistuba, V. Schurig, *J. High Res. Chrom. Chrom. Commun.* **1989**, *12*, 383.
[22] J. Mraz, L. Feltl, E. Smolkowa-Keulemansova, *J. Chromatogr.* **1984**, *286*, 17.
[23] G. Fabian, A. Knoll, F. Theil, M. Böhme, in Vorbereitung.
[24] K. Grob, 'Making and Manipulating Capillary Collumns for Gas Chromatography', Dr. Hüthig Verlag, München, 1986, S. 156 ff.
[25] F. Theil, H. Schick, M. A. Lapitzkaya, K. K. Pivnitzky, *Liebigs Ann. Chem.*, im Druck.
[26] P. A. Grieco, *J. Org. Chem.* **1972**, *37*, 2363.

COMPUTATIONAL CHEMISTRY COLUMN

Column Editors:
Prof. Dr. J. Weber, University of Geneva
PD Dr. H. Huber, University of Basel
Dr. H. P. Weber, Sandoz AG, Basel



Editors' Note

We would like to remind our readers that their contributions to this *Column* are most welcome, in the form of comments, letters, *etc.*, relating to any topic of general interest in computational chemistry or to the subjects presented in previous issues. It is indeed one of the main purposes of the *Column* to be a forum where, in addition to the publication of general articles, ideas could be exchanged and, would it be the case, debated for the sake of providing new information to our readership.

Chimia 45 (1991) 198–199

Computational Chemistry in Switzerland and the Future HLR-91 Supercomputer

All Swiss scientists, and chemists are no exception, specialized in supercomputing are aware of the developments of the HLR-91 (HLR = Hochleistungsrechner) project. However, in view of its importance and the new possibilities it offers to Swiss computational chemists, we found it worthwhile to present and discuss the HLR-91 project in some detail in this Column, keeping in mind that most of our readers are probably not specialized in (super)computers.

All the story started a few years ago when the Swiss federal parliament voted a budget of 40 Mio SFr. for encouraging and developing the use of supercomputers by the universities and federal institutes of technology of our country. This gave birth to the so-called HLR-91 project consisting essentially in the acquisition of a third HLR in Switzerland (in addition to the CRAY-YMP and CRAY-2 machines installed at ETHZ and EPFL, respectively) and to have it functioning in the early nineties. There is no doubt that this project is both important and timely, as high-level research in several fields can no longer be achieved without resorting to large-scale calculations on supercomputers with performance rates of the order of 100–1000 Mflops (1 Mflop = 1 million floating point operations per second). It is indeed a truism to state that supercomputers have become indispensable in the following applications (the list being not exhaustive):

- computational fluid dynamics (*e.g.* turbulence and combustion processes)
- structural analysis (*e.g.* crash simulation)
- wheather forecasting and climate research
- quantum chemistry and macromolecular modelling (*e.g.* drug design and protein folding)
- materials science (*e.g.* new high-T_c super-conductors)
- plasma physics
- seismic explorations.

There was, therefore, every reason to believe that the research projects undertaken in these fields and in progress in Swiss universities and ETHs would also take advantage of supercomputing facilities, and the Swiss parliament and high authorities should be thanked for having initiated the HLR-91 project. So, today, five years after the installation of the first supercomputer in Switzerland (CRAY-1S at EPFL), where are we going with HLR-91?

After many years of long discussions within several *ad-hoc* committees (under our latitudes, the decisional procedures are always slower than one would normally expect), the final decisions concerning HLR-

91 were known in the second half of last year: a new Swiss center for scientific computation (Centro svizzero di calcolo scientifico (CSCS)) will be opened in Manno nearby Lugano and the supercomputer to be installed there is a Japanese machine marketed by NEC Corporation (Tokio): the SX-3. In its initial configuration, the SX-3/Model 22 supercomputer will have two CPUs with a peak performance rate of 2.75 Gflops each (1 Gflop = 10^3 Mflops), and it is planned that the machine will be upgraded in the near future so as to have a peak performance rate as high as 22 Gflops. The SX-3 supercomputer is scheduled for installation in Manno in summer 1991 and it should be available to its first users next September.

Broadly speaking, it is good news that the HLR-91 project has entered now its final stage, and that a new machine with such an impressive compute performance will soon be available to the Swiss scientific community. However, if everybody agrees on the principle, the choice of the machine which finally prevailed for HLR-91 has raised some concern among part of that community. This supercomputer will be among the first ones of this type to be exported from Japan, and little is known about the availability of the numerous highly vectorized and multi-tasked application softwares required by scientists so as to take the maximum advantage of the enormous computing capability of this machine. This is in contrast with some other manufacturers, such as CRAY Research, which have sold for many years hundreds of supercomputers all around the world, and which offer an impressive list of performing application software. We should open here a parenthesis for the innocent reader: the special architecture of any type of supercomputer requires professional skill and important programming effort, when a user wants to take full advantage of the high power of the machine. Efficient programming on a supercomputer resembles program development on a personal computer as much as driving a F1 car resembles sitting at the wheel of the car of 'monsieur tout le monde'.

Coming back to HLR-91, this concern was expressed by the Group of Swiss Computational Chemists (GSCC) which comprises *ca.* 70 members both from academia and industries. In a letter sent to Prof. *J. Nüesch*, president of ETHZ, and to the persons in charge of negotiating the contracts with NEC, the GSCC pointed out that the availability of adequate application software in chemistry is essential for an efficient use of such a machine and that chemists generally do not have the time nor the skill (without mentioning copyright problems for commercial packages!) for a transport of their programs from the existing CRAYs to the NEC. According to the GSCC, these problems were seriously to be taken into account, because as much as 30% of the resources of the two CRAYs were devoted last year to computational chemistry applications. In addition, the question of adequate users support in Manno was raised by the GSCC.

In a long and detailed answer, Prof. *Nüesch* explained that a fair and efficient repartition of the total resources available on the three Swiss HLRs would be performed and that users lacking for adequate software on the SX-3 would be allowed for many years to continue working on the existing CRAYs. However, this is only possible, if most new applications requiring CPU time on HLR take place in Manno, and several existing ones are transported to the SX-3 as well, enabling thus users without proper software for that machine to work on the CRAYs. In addition, Prof. *Nüesch* mentioned that the availability of application software in computational chemistry would be part of the contract to be negotiated with NEC, which is in our opinion an essential point.

Finally, concerning the users support in Manno, the problem is that the staff of the GSCC will be limited to 19 people altogether, which means that users support will be minimal. In this respect, the position of Prof. *Nüesch* is that Swiss universities and ETHs should try to organize their own support, which will be difficult to set up for both financial and staff limitation reasons.

In its last meeting, held March 20th 1991 in Bern, the GSCC discussed the present situation concerning HLR-91. It was the participants' opinion that the reassuring answer from Prof. *Nüesch*, mainly as far as the availability of computational chemistry software is concerned, enables them to be pretty optimistic about the possible use of the SX-3 for their applications. Indeed, it was reported during the meeting that in principle several packages should be available next fall: mathematical libraries, a graphic library and, as far as we are concerned, computational chemistry (AMBER, AMOSS, semi-empirical programs, *etc*...). Concerning the popular GAUSSIAN package, the question is still open and it seems impossible to make yet accurate previsions as to the date it will be available.

As to the practical access to the SX-3 machine, two 2 Mbauds (1 Mbaud = 10^6 bit per second) lines will be made available by the PTT between Manno and the ETHZ and EPFL, respectively. It is planned that in the future these lines will be upgraded to 34 Mbauds, which should be adequate for applications requiring extensive data transfer, such as graphics.

Though the programs to be initially installed represent undoubtedly the 'vital minimum' in computational chemistry, one may say as a conclusion that the perspectives offered to chemists by the HLR-91 project are promizing and allow to be rather optimistic as to the possibility to perform large-scale molecular dynamics simulations or quantum chemical calculations on the SX-3 machine. However, many problems remain to be solved, before computational chemists can really start to explore and possibility exploit the enormous compute power of this new supercomputer.

Chimia 45 (1991) 199–202

Import of Chemical Information into Word Processors

Heiner G. Bührer*

Abstract. Instead of drawing curves and sketches by hand and cutting and pasting pieces of paper containing chemical information, it is often easier and gives professional-looking results to perform evaluation and representation of data with specialized software. The resulting file can be imported into a suitable word processor. How this can be done with the help of some popular *MS-DOS* programs is described in the article.

1. Introduction

The way chemists write publications has changed significantly in the last 20 years. Three periods can be distinguished:

– *The period of the typewriter, the pen, and the ruler*: The chemist wrote his (or her) article once or several times by typewriter, added chemical and mathematical formulae by hand, made drawings of his equipment and plotted curves from his (analogous) measurements. Sometimes, a secretary could

**Correspondence*: Prof. Dr. H. G. Bührer
Industrielle Chemie, Chemieabteilung
Technikum Winterthur Ingenieurschule
CH-8401 Winterthur