

## FOREWORD

The MATH/CHEM/COMP 2000 (MCC 2000), the Fifteenth Dubrovnik International Course & Conference on the Interfaces between Mathematics, Chemistry and Computer Sciences, was held at the Inter-University Centre, in Dubrovnik, Croatia, on June 19-24, 2000, under the joint auspices of the Inter-University Centre, Dubrovnik, Croatia, Ruđer Bošković Institute, Zagreb, Croatia, Universities of Zagreb & Split, Croatia, International Society for Mathematical Chemistry, and International Society for Theoretical Chemical Physics.

The morning of the first day of MCC 2000 was devoted to mathematics in art, history and sciences, and the afternoon to discrete mathematics and topology in chemistry and physics. The morning sessions of the second day, June 20, were dealing with mathematical chemistry and physics as well as computation and modelling in science and technology. The lectures on the latter topic continued during the afternoon session. Special sessions on advanced materials held on Wednesday morning, June 21, and Friday afternoon, June 23, covered new achievements in chemistry and physics of materials. This mini-symposium was organized by Zorica Crnjak Orel, Ante Graovac, Edward C. Kirby, Stane Pejovnik, and Aleksandra Turković. On Thursday, June 22, a special session on proteins, bioinformatics and biocomputing was organized by Davor Juretić, Gabor Naray-Szabo, and Nenad Raos. The morning session on Friday, June 23, was devoted to chemical structure and reactivity. Special PLIVA d.d. session on recent advances in drug design, organized by Vesna Gabelica, Adalbert Kerber, Tom Šolmajer, and Ivar Ugi, took place on Saturday, June 24. The MCC 2000 meeting attracted a hundred participants from fifteen countries, a large number of them being students and young researchers.

Part of the results presented in the above mentioned sessions are published in this special issue of *Croatica Chemica Acta*. Other papers from the MCC 2000 will appear as a special issue of the *Journal of Chemical Information and Computer Sciences* in 2001.

The organization of MCC 2000 was possible in the first place due to the help of the Inter-University Centre in Dubrovnik, Ruđer Bošković Institute, Zagreb, University of Zagreb, and University of Split. The financial support of the Ministry of Science and Technology of the Republic of Croatia and PLIVA d.d. (Zagreb) is gratefully acknowledged. Special thanks for partial financial support go to the COST, the German Academic Exchange Service (DAAD), City of Dubrovnik, Open Society Institute (Zagreb), Agencija za posebni otpad-APO (Zagreb), CEE (Ljubljana, Slovenia), Croatia Airlines (Zagreb), Dr. Etlinger d.d. (Zagreb), Herba Dalmatica (Split), Krka (Novo

Mesto, Slovenia), Sava Tires (Kranj, Slovenia), SMS (Split), Splitska banka (Split), Velinac d.d. (Sesvete) and WET d.o.o. (Zagreb).

The Third International Dubrovnik NMR Course and Conference, DU 2000 NMR, was held on June 26-July 01, 2000, at the Inter-University Centre in Dubrovnik, Croatia, under the joint auspices of the Inter-University Centre, Dubrovnik, Ruđer Bošković Institute, Zagreb, and Faculty of Food Technology and Biotechnology, University of Zagreb, Croatia. The meeting attracted more than eighty participants from Croatia and seven other countries.

The first and the second day of the DU 2000 NMR were devoted to the nuclear magnetic resonance of biomolecules, especially proteins. Lectures were presented by Nenad Juranić, Vladimir Sklenar, Roman Jerala, Simona Golič Grdadolnik, and Sanja Tomić. On Wednesday, June 28, the past, present and future of NMR spectroscopy in Croatia was reviewed by Dražen Vikić-Topić. In the morning on Thursday, June 29, lectures on cross-correlation effects, conformational analysis of natural products and CP-MAS of transition metal complexes were delivered by Norbert Müller, Predrag Novak, and Yuri Oprunenko, respectively. In the afternoon of the same day the application of NMR in food science was presented by Jurka Kidrič. During the last day of the meeting different NMR topics were covered: structural analysis of saponines by Ernst Haslinger, clustering and proton exchange in water by Nicolay Sergeev, isotope effects in NMR by Nicolay Sergeev and Dražen Vikić-Topić, and NMR problem solving by Milena Jadrijević-Mladar Takač. Some of the results presented at the DU 2000 NMR are published in this issue of *Croatica Chemica Acta*.

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Ante Graovac (Zagreb & Split)  
Dražen Vikić-Topić (Zagreb)

## SAME TIME NEXT YEAR IN DUBROVNIK, CROATIA

In June of Y2K,  
I'm sorry I must say

Dubrovnik won't see me  
Because then I must be

First of all in Greece,  
Not to talk on peace,

But at an economics meeting.  
My talk will be worth repeating,

Using graph models of course  
In a code that isn't Morse.

The next conference is in Romania,  
Constanca on the Black Sea  
Will be its location. There we  
Will go swimming with gusto and mania.

Although I love mathematical chemistry  
In every field there is some sophistry.

Still the subject is so beautiful  
That research is nowise dutiful.

Scholars work here for pure joy,  
Like playing with a funny toy.

Hence I congratulate you all  
For doing work like having a ball,

This is my welcome to all of the participants at the 2000 meeting.  
I look forward to seeing you all in person next year,  
where there is sure to be adequate seating.

In 2001 I'm due to become 80,  
But my lecture then will be light, not weighty.

I do not know to be unclear or boring  
As an eternal optimist, my hopes are always soaring.

What happiness there will be  
To hear you all sing »Happy Birthday« to me!

Frank Harary, Las Cruces, New Mexico, 2000