

## GREETINGS AND REMINISCENCES

My strong links with Croatian theoretical chemistry started from my friendship with Milan Randić when we were both members of Corpus Christi College in Cambridge at the end of the 1950s. This continued when Milan came to spend a year with me at Sheffield University and I made a visit to Rugjer Bošković Institute. One of the papers I wrote in my last year at Cambridge was on the wave functions of hybrid orbitals, and how these were best defined when they were not determined by symmetry; the method was based on Linus Pauling's observation that symmetry-determined hybrid orbitals (*e.g.* for methane) had maximum overlap with ligand orbitals. Milan and I were working on intermolecular forces

when he was in Sheffield but we used to chat about maximum overlap hybrids, and on his return to Rugjer Bošković Institute, he proposed this topic for Nenad Trinajstić's MSc thesis; I naturally took a great interest in how the topic developed.

I have been lucky at several periods in my research career to have a little money with few strings attached, and I always tried to use it for overseas students; without exception this money has been well spent. Milan suggested that Nenad should spend a couple of years with me at Sheffield, and he arrived in the autumn of 1964. Sheffield in those days was a rather dreary city, particularly in winter, and I think his wife Judita, who came



Theoretical Chemistry Barbecue at Newtimer (John Murrell's house) in June 1966.

Sitting in front: John Murrell, Janice Carter (secretary); Standing in the first row: Keith Miller, Nenad, Yoshiya Harada, Martin Lloyd, Bob Ditchfield, Ruth Lynden-Bell, Gil Jones, Vic Saunders, Brian Pedley, Edward Bishop; Standing in the second row: Phil Stevenson, John Stamper, John Fleming, Matthew Jensen, Alan Tweedale, Stuart Carter.

with Nenad, must have been a bit dispirited with the situation. However, the physical chemistry department under George Porter was an intellectual hot spot, and I was lucky to have a large group of PhD students doing theoretical chemistry. To say that Nenad fitted well with the group is an understatement; the continuing academic links and friendships he maintained with my other students is testimony to that. As well as papers he published with me, he published joint work with Stuart Carter and Alan Hinchliffe.

One of my criteria for a good scientific researcher is that they move away from the topics they worked on for their PhD. Nenad and I were mainly interested in the electronic states of aromatic molecular ions (the topic of his PhD thesis when he returned to Zagreb), and when he moved with me to Sussex University we did a little

work on localised orbitals. But later he did an enormous amount of work when he was in Texas, extending and applying Dewar's MINDO programs, and after that he became a leading figure in mathematical chemistry, particularly topics based on graph theory.

My contribution to this celebration issue is rather outside the normal topics covered by CCA, but it is not outside Nenad's interests. In the last few years, as my attention has moved to the historical development of physics and chemistry, I have had many stimulating discussions, and exchange of e-mails, with Nenad on these matters; while I am still a beginner in this area, he has a scholarly background that I may never catch up.

I can do no better than wish us both many years of mutual scientific interests and friendship.

*John Murrell*

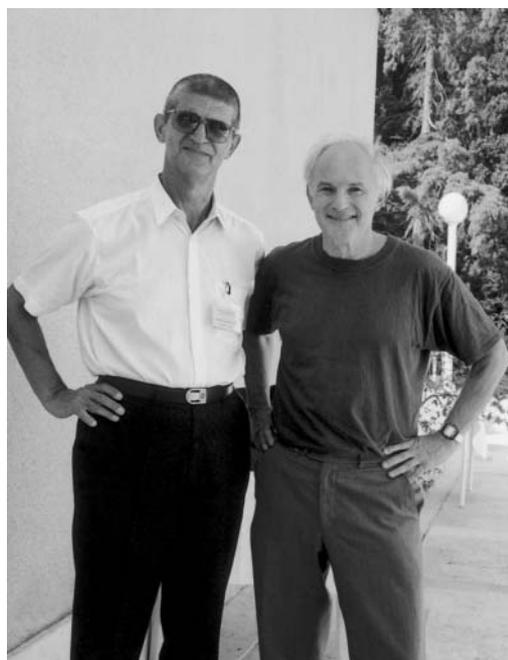
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*Professor John N. Murrell FRS  
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It is an honour and pleasure to write some short notes for this volume dedicated to Nenad whom I have known ever since our paths first crossed in Sheffield many years ago in the 60s when life was so much much simpler. A long line of Rugjer Boškovićians has made the pilgrimage from Zagreb either to Sheffield or Sussex or often both where John Murrell created Theoretical Chemistry Meccas. A very special relationship with the Rugjer Bošković Institute was created as scientists from Croatia and the UK journeyed backwards and forwards. Milan Randić, Nenad, Danko Bosanac, Tomislav Živković, Alka Velenik all came to the UK. My first meeting with one of these invaders from the Balkans was with Milan Randić who introduced me not only to the vibrational theory of molecules but also the well-known Croatia custom of non-stop joke-telling until the early hours of the morning. Indeed as the nights wore on, the jokes became less and less readily re-tellable in polite company. As more-and-more visitors from the Rugjer Bošković Institute came and went, I came to realise that the endearingly gregarious nature, the ability to tell great jokes, the good company and the wide range of interesting conversation ranging across science, politics, history all generously embellished by good food and wine was a general characteristic of visits to Zagreb. Nenad has been at the heart of this activity and has made very important contributions to maintaining a scientifically and socially rewarding relationship.

It also seems to me that at least two areas of my research work benefited serendipitously from the areas that Nenad and co-workers have pioneered. The first area relates to our carbon chain molecules in space where an understanding the vast range of possible isomers which might exist in space benefited from the chemical structure organisational approaches that Nenad developed. When the Fullerenes were discovered it was clear that again the theoretical methods which could organise the vast numbers of species and in particular the electronic configurations had at last met up with a molecules worthy of the techniques that had been developed. Related methods were invaluable aids to understanding on a sound theoretical basis the structural reasons for the special nature of  $C_{60}$  and its side-kick  $C_{70}$ . At the time the result provided the most compelling »proof« that the closed cage Buckminsterfullerene structure for  $C_{60}$  was correct.

Croatians can claim with good reason that Rugjer Bošković was the father of chemistry as he was the first to draw a potential curve for particle particle interactions. Historically an amazingly prescient concept. Indeed the great scientist Richard Feynman has indicated that he thinks that the potential curve for chemical bond is the most important idea ever. Nenad has spent his research life developing similarly elegant ideas and applying them to important problems in chemistry. In this way he and his colleagues follow in the footsteps of Rugjer



Professor Sir Harold W. Kroto FRS and Nenad Trinajstić at the Brijuni Conference 2002 (Brijuni, Croatia: August 26–30, 2002).

Bošković. On a personal level it is a pleasure to pay tribute to Nenad and his efforts to help make Zagreb and in particular the Rugjer Bošković Institute such pleasant and stimulating place where not only can one do excellent science but also build friendships that last a lifetime. I thank Nenad and his many colleagues at the Rugjer Bošković Institute for introducing me to Croatia, Zagreb and last but not least to good Croatian food and vines.

Harry Kroto  
16-6-2003 Sussex

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Dear Trina,

It gives me great pleasure to wish you all the best on the occasion of your 65<sup>th</sup> birthday and forty years of remarkable scientific activity. You can feel justly proud of both anniversaries, and we all celebrate them together with you. Your name will always be inseparable from the birth and the development of theoretical chemistry in Croatia. But, the impact and the recognition of your activities as a scientist and mentor to a whole new generation of theoretical chemists extends far beyond the borders of Croatia.

It is safe to say that through your lectures and books on quantum chemistry, as well supervision of undergraduate and graduate students, you have left an indelible mark on just about every younger Croatian physical and theoretical chemist, many of whom are scattered around the world. This was certainly the case with me. The year of undergraduate research with you a quarter of a century ago, and your strong recommendation that enabled me to pursue graduate studies in the US, have shaped my life ever since. Your integrity, high standards, and dedication to science, has always been an inspiration to me.

Dear Trina, live long and continue to work and write; for you, this is one and the same. Let us all gather for your 70<sup>th</sup> birthday, to begin with, and then for the 80<sup>th</sup>,.....



Professor Zlatko Bačić and Nenad Trinajstić in Greenwich Village (New York City) during Trinajstić's visit to New York University in the spring of 1988.

Yours,  
Zlatko

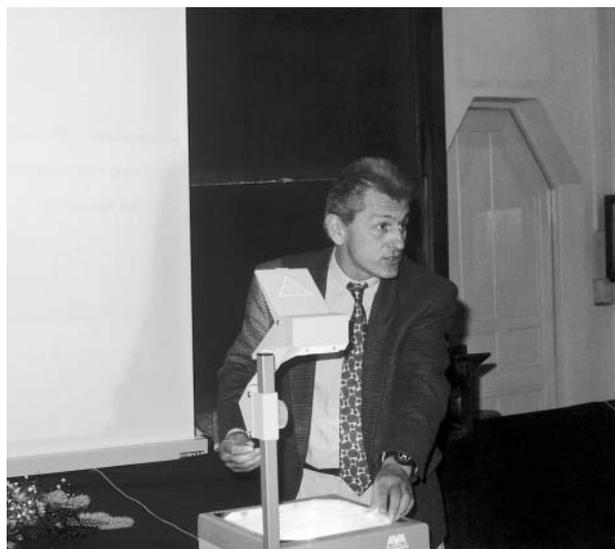
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Prof. Trinajstić came back from Austin, Texas, to Zagreb, after spending two years with Prof. Dewar, to find me sitting in his office and calculating matrix elements for the norbornane molecule in the Extended Hückel Molecular Orbital approximation, the chore given to me by prof. Randić, who had in the meantime left Zagreb for good. »I am Trina«, he said, »You must be Milun. I have a nice and easy problem for you. A simple Hückel description of aromaticity. Small matrices and easily solved. Are you interested?«. I was. It was in 1970. Early in 1971 Trina pushed me to give a talk at the Croatian Chemical Society meeting in Zagreb and only one year later made me deliver a twenty minute talk at an international meeting in Bucharest. For a recently graduated young man like I was at the time it was a terrific experience. This nicely illustrates the essentials of Trina's pedagogical method: accept every person interested in science, give her or him a chance, encourage, push from time to time and most of all publish the results. It was very important for me to have such a mentor in those formative years, for Trina treated all of his students as peers, delivered criticism and accepted it without hard feelings. The Theoretical Chemistry Group at the Rugjer Bošković Institute was very young in those years: Trinajstić, Maksić and Klasinc were seniors (as they still are), Graovac, Živković, Kovačević, Gutman and Milun were postgraduate students and the agenda included theoretical chemistry, quantum physics, science in general, literature, philosophy, politics, *etc.*, is-

sues feverishly discussed at group seminars, lunch breaks, walks through Rugjer's park, in various inns and at many parties. If our seniors were different, such an atmosphere would not have been possible and we ourselves would probably develop different professional personalities. Trina was an essential ingredient in my scientific development and I greatly appreciate his friendship and leadership in those times.



Milorad Milun giving a talk at the day-symposium on the occasion of the 60<sup>th</sup> birthday of Nenad Trinajstić (Zagreb: October 25, 1996).

*Mišo*  
June 16, 2003

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*Dr Milorad Milun*  
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*Bijenička c. 46, 10 000 Zagreb, Croatia*

Dear Trina,

I am writing this letter after it became certain that I will not be able to come to Dubrovnik, to participate in the festivities on the occasion of your 65<sup>th</sup> birthday and 30 years long (or longer?) fruitful research in Chemical Graph Theory. I was supposed to say a few words there. Let these lines serve as a substitute for what I intended to say.

Dear Trina, dear teacher, dear friend

Let me begin by quoting from a paper, published quite some time ago:

For everything its season, and for every activity under heaven its time:... a time to scatter stones and a time to gather them;

So, the time has come, for both you and me, to re-collect, to summarize, to conclude, to gather. How far is now the Spring of 1971 when young Gutman arrived to Zagreb, determined to study theoretical chemistry? When he was directed to the Rugjer Bošković Institute, when it happened that you were the only theoretical chemist present at the moment, when you mentioned to him a problem which he was able to solve analytically in Summer 1971, staying in his native town Sombor [Gutman, Milun, Trinajstić, *Croat. Chem. Acta* **44** (1972) 207]. How naive and inexperienced we all were in Spring 1972 when we submitted the first joint paper on (what is nowadays called) Chemical Graph Theory [Graovac, Gutman, Trinajstić, Živković, *Theor. Chim. Acta* **26** (1972) 67]. How little we knew then, and how much we have learned since then. How long is the trail we have passed.

Whichever the metric we use, we must accept the sad fact that the length of the trail passed exceeds the length of the trail ahead of us. Then we may ask: what we have left behind us?

What have you, dear Trina, left behind you?

As far as I know, there is no Trinajstić rule, no Trinajstić theorem, no Trinajstić algorithm, no Trinajstić determinant and no Trinajstić index. You did a bit more: after you published your book *Chemical Graph Theory*, the entire scientific world has accepted the name Chemical Graph Theory for the respective part of theoretical chemistry.

Today: I am doing research in Chemical Graph Theory; you, he, she, we and they are doing research in Chemical Graph Theory.

There is something more: You had scores of students whom you taught how to do scientific research. It happened that I was one of the first among them. Now, as someone else said:



Judita Trinajstić and Professor Ivan Gutman during the coffee break at the ISNA 4 – Fourth International Symposium on the Chemistry of Novel Aromatic Compounds (Jerusalem: August 30 – September 4, 1981). In the background are Mrs Vogel, wife of Professor Emanuel Vogel of the University of Cologne, and Professor B. Andy Hess, Jr. of Vanderbilt University in Nashville.

A sower went out to sow his seed. And as he sowed, some seed fell along the footpath, where it was trampled on, and the birds ate it up. Some fell on rock and, after coming up, withered for lack of moisture. Some seed fell in among thistles, and the thistles grew up with it and choked it. And some of the seed fell into good soil, and grew, and yielded a hundredfold.

The assumption behind this parable is that the number of seeds (the seed count, SC) is sufficiently large (»whatever sufficiently large means« – to use a saying I learned from you). Well, your SC (= student count) is so large that a non-negligible number of them fell into good soil.

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It is said that there is no greater happiness for a teacher than when his student becomes greater than him. Well, Trina – in my case you should be a very happy man. I am now much bigger than you are: I weigh over 130 kg and I am still improving my performance. In fact, I may be the biggest of all of your former students. If not – I will know what to do.

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You wrote so many papers in so many areas of science, culture, literature,... that I don't even dare to conjecture a reasonable lower bound. Let me use this occasion to ask you for a favor. A favor not to me, but to the Croatian scholars-to-be (around the middle of this century, say): Don't reveal the number of your papers, don't publicize a complete list thereof. Think of the Ph.D. theses written around year 2050, entitled »Nenad Trinajstić's

chemical papers«, »Analysis of a few newly discovered papers by Nenad Trinajstić«, »An attempt to complete Nenad Trinajstić's publication list«, »Towards Nenad Trinajstić's collected works«.

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Ending this letter, I quote again an early author:

One further warning my son: the use of books is endless, and much study is wearisome.

So, Trina, maybe the time has come to live a less serious and more relaxed life, to enjoy the fruits and to sit watching how the new generation destroys and overcomes all that we have tried to build.

The time has come, my dear Trina,  
to talk of many things:  
Of shoes and ships and sealing wax  
Of cabbages and kings.  
And why the sea is boiling hot  
And whether pigs have wings.

See you at your next anniversary! Cheers!  
1 joint book with N.T. &  
52 joint scientific papers with N.T. &  
10 joint expert papers with N.T.

*Ivan Gutman*

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