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Recollections about Professor Oskar E. Polansky: A Personal Account Occasioned by the 30th Anniversary of MATCH

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Introduction

Thirty years ago, in May 1975, the first peer-reviewed periodical dedicated to publishing papers in the field of mathematical chemistry (*Informal Communications in Mathematical Chemistry, (*MATCH*)* was founded. The first word of the title was dropped in 1980. It had four editors (in alphabetical order: A. T. Balaban, A. S. Dreiding, A. Kerber, and O. E. Polansky), and was published by the Max-Planck-Institut für Strahlenchemie in Mülheim an der Ruhr, Federal Republic of Germany. The main editor was **Oskar E. Polansky**, who was also one of the two Directors of the host Institute.

Brief sketch of Oskar E. Polansky's life and activity

It may be appropriate to recall a few biographical data about Professor Polansky, including information on his connections with Vienna and Mülheim. More detailed accounts may be found in ref. [1]. Born in 1919 in Vienna, he studied chemistry at the University of Vienna (1947-1953) but during the Second World War he was drafted and served in cavalry. He resumed his studies at the end of the war, and he worked during 1953-1957 for his Ph. D. Thesis under Professor F. Wessely on 1,2- *versus* 1,4-addition of Grignard reagents or phenyllithium to α,β-unsaturated carbonyl derivatives related to quinones. After a post-doctoral stay in Oxford for several months with Professor C. A. Coulson, he could explain the experimental results he had observed by carrying out quantum-chemical calculations. In all his subsequent research, Professor Polansky maintained this equilibrium and reciprocal stimulation between experiment and theory. His "Habilitationsschrift" in the area of Theoretical Organic Chemistry followed in 1963. He was appointed as Adjunct Professor (Extraordinarius) for Theoretical Chemistry in 1965, and then in 1967 as full Professor (Ordinarius) and Chair Director (Vorstand des Instituts für Theoretische Chemie) at the Vienna University. He maintained this position

till 1973, when he resigned in order to make fewer trips between Vienna and Mülheim an der Ruhr. Since 1965, he had been a regular guest scientist at the Max-Planck-Institut für Kohlenforschung (MPIKF) in Mülheim, which had become famous and very prosperous owing to patent royalties earned by its director (K. Ziegler who had received the Nobel Prize together with G. Natta for discovering the low-pressure polymerization of ethylene and the stereospecific polymerization of propene). Professor Polansky's research on stable organic electrically-neutral Lewis acids (obtained from the reaction of aldehydes with Meldrum's acid, i. e. with isopropylidene malonate or 2,2,-dimethyl-1,3-dioxane-4,6-dione) led him to investigate the cycloadditions of these methylene-derivatives of Meldrum's acid: 1,3-dipolar cycloadditions, Diels-Alder reactions with electron-rich dienes, and photochemical cycloadditions yielding cyclobutane derivatives. It was owing to this involvement in photochemistry that in 1968 Professor Polansky became a Scientific Member of the Max-Planck-Institute for Carbon Research (MPIKF), which had an Independent Section for Radiation Chemistry, whose Director he became in 1970, sharing responsibilities with Professor D. Schulte-Frohlinde. In 1973, this Section became "Institut für Strahlenchemie im Max-Planck-Institut für Kohlenforschung", and in 1981 it obtained today's rank of "Max-Planck-Institut für Strahlenchemie" (MPISC). Since 2003, the name has changed into "Max-Planck-Institute for Bioinorganic Chgemistry". In 1974-1976 and 1983-1985, Professor Polansky was Managing Director. However, he continued to give lectures to students, obtaining the title of Honorary Professor from Universities in Dortmund (1973) and Vienna (1984).

The major scientific contributions of Professor Polansky in theoretical chemistry are the development of the Pars-Orbital-Method (allowing to find a measure of local aromaticities in benzenoids or of diene character in their bay regions, augmenting quantitatively Clar's theory), and of the Topological Effect on Molecular Orbitals that explains the interlacing of absorption bands in UV-Vis and photoelectron spectra.

As Co-Director of the MPISC, Professor Polansky had the possibility of acquiring numerous coworkers and of inviting foreign scientists, especially from Yugoslavia, Bulgaria, and Romania (the difficulty of traveling abroad increased in that order). From Yugoslavia, he collaborated with Drs. A. Graovac and I. Gutman, the present Editor of MATCH. With him, he published the book "*Mathematical Concepts in Organic Chemistry*, Springer Verlag, Berlin, 1986. From Bulgaria, he collaborated with Drs. D. Bonchev and N. Tyutyulkov on graph-theoretical problems and properties of polymers. From Romania, he invited Prof. C. Nicolau and Dr. I. Moţoc for longer periods, and me for shorter stays.

My first encounter with Professor Polansky

Professor Polansky's name was well known to theoretical and organic chemists in September 1966, when I arrived in Austria as a United Nations civil servant at the International Atomic Energy Agency (IAEA) in Vienna, with the position of Senior Research Officer (P5) in the Chemistry Section of the Division of Research and Laboratories. At that time, I was an Associate Professor of Organic Chemistry at the Bucharest Polytechnic on leave of absence, but I continued to be the Head of the Laboratory of Isotopically Labeled Organic Compounds in the Institute of Atomic Physics, Bucharest, Romania. I became familiar with my duties in the IAEA (organizing

international meetings on the preparation and quality control of radioisotopes and radiopharmaceuticals, and editing books in this field). Being also trained as an organic chemist after having obtained my Ph. D. degree with Professor C. D. Nenitzescu in Bucharest, and having an interest in theoretical chemistry (especially graph-theoretical applications), I tried to make contacts with the Chemistry Departments in the Vienna University and Technical University (TH). I attended their seminars, and I recall a lecture held at the TH by Professor J. Bestmann from West Germany, who was introduced by the host, Professor Viktor Gutmann, the Chairman of Inorganic Chemistry with the remark to the audience: you see how inorganic chemistry compares with organic chemistry by noting that I am "der anorganiker Gutmann", but our lecturer tonight is "der organiker Bestmann".

I obtained permission to carry out some chemical experiments in the IAEA Laboratories in the Nuclear Center Seibersdorf, in the proximity of Vienna. However, for ^{1}H-NMR spectra I gave my compounds to Dr. W. Silhan at the Institute of Organic Chemistry of the Vienna University in Währingerstrasse. We published together two papers [2]. Also, my wife obtained permission to work for her Ph. D. thesis in Chemical Engineering at the TH Vienna, when the grandparents of our son and daughter were visiting us, and acting as baby-sitters.

During these contacts, I had the pleasure and honor of meeting Professor Oskar Polansky, a friendly and erudite chemist and a perfect gentleman, who invited my wife and me to dinner at restaurants, and then after dinner, for an extra bottle of wine at his home. He had been interested at that time in quantum-chemical calculations involving molecules that had hydrogen bonds. I discussed with him about the graph-theoretical problems that I had studied in Romania and that continued to interest me. We maintained contact by letter after 1970, when I returned to Romania. Around that time, in addition to quantum-chemical problems, Professor Polansky developed an interest in solving structural problems that did not involve number crunching, but a graph-theoretical approach. He grouped around him persons sharing these interests such as post-doctoral fellows (such as Ioan Moţoc, who had taken with me his Ph. D. thesis, and Dennis Rouvray who had been a Professor at the Witwatersrand University in South Africa).

Launching the *Communications in Mathematical Chemistry,* (MATCH)

In May 1975, a Micro-Symposium presided by O. E. Polansky on "Graph Theory in Chemistry" was sponsored by the Max-Planck-Institut für Strahlenchemie. The 36 participants from seven countries complained about the difficulty of having their papers accepted in mainstream journals (this difficulty still persists to some degree) and proposed the foundation of a journal dedicated especially to this area of theoretical chemistry.

At the initiative of Professor Polansky, together with André Dreiding from Zürich, Adalbert Kerber from Bayreuth and me, we issued in 1975 the first peer-reviewed journal (*Communications in Mathematical Chemistry,* MATCH) dedicated to publishing papers in the field of mathematical chemistry (at first with an informal character, and soon afterwards as regular articles).

After Professor Polansky passed away in 1989, it was thanks to Professor K. Schaffner, who had taken the Director position for MPISC, that the publication of

MATCH could continue. One should also acknowledge the contribution of Dr. H. J. Kuhn and of the secretary Mrs. Renate Wolf, who helped in the production and distribution of MATCH.

In 1976 the first book on chemical applications of graph theory finally appeared [3]. I had started editing it during my stay in Vienna, and continued after my return to Bucharest, but it was more and more difficult to correspond with the contributing authors due to the political restrictions. One of the authors (contributing with the chapter on the topological matrix in quantum chemistry) was Dennis Rouvray, who had published excellent reviews [4] on graph-theoretical applications in chemistry.

Clouds over and life in general, and especially over scientific research, in Romania

After my return from Vienna to Bucharest, the situation under the dictatorship of Nicolae Ceauşescu with his wife's (Elena Ceauşescu) oppressive domination of all scientific life in Romania became gradually less and less tolerable. Food became scarce, homes became cold in winter (in 1985, no heat being supplied to most of Bucharest, including our centrally-heated apartment, the water in heating elements froze and the metal burst, so that my wife and I had to move and stay for a few months in our son's two-room apartment, where he lived with his wife and daughter).

My travels abroad to scientific meetings where I was occasionally invited to present plenary lectures had to be personally approved by Elena Ceauşescu (like travels abroad of any member of the Romanian Academy; I was a corresponding member, and I was not promoted to titular member during the Ceauşescu regime). My wife was no longer allowed to accompany me on the rare occasions when I was able to travel abroad during the Ceauşescu regime.

In Bucharest, experimental organic chemical research in the Polytechnic University had to overcome three hurdles: lack of chemicals (our undergraduate and graduate students helped by performing long syntheses starting with simple reagents), lack of instrumentation (my first papers on spectral characterization of pyrylium salts [5] were co-authored with chemists from other laboratories in Romania or abroad), and lack of documentation, namely books and periodicals. Whereas the first two handicaps could be overcome as indicated above, the third one was the most difficult: one had to rely on asking for reprints from the authors, and when they failed to reply, from friends abroad. This third type of hurdle applied also to theoretical work, towards which I turned more and more because it was easier to carry out by myself alone, as I never had a large group of coworkers.

Events that seem taken from Eugen Ionescu's or Samuel Beckett's *Theater of the Absurd*, but were tragicomic when they happened

To give just a few examples of the difficulties we had to face, I shall include a few events that would fit a theatrical representation authored by the Romanian writer who migrated to France and was known by his French-sounding name Eugène Ionesco. In Romania there was one more chemist who shared my interests in theoretical chemistry,

namely Dr. Zeno Simon. He had graduated from Bucharest University and had obtained a Ph. D. degree with a thesis in physical chemistry with Professor I. G. Murgulescu. At that time Romanian chemistry in Bucharest had two towering figures; both were titular members of the Academy: C. D. Nenitzescu at the Polytechnic Organic Chemistry Department (he had been my Ph. D. supervisor), and I. G. Murgulescu at the University Physical Chemistry Department. With Z. Simon, who had become a professor of Biophysics at the Medical School in Timişoara, we collaborated on several papers, and some of his students were directed to me for Ph. D. topics. One of them, Ioan Moţoc, was my best graduate student in theoretical chemistry, but unfortunately, after his emigration to USA and his divorce, he died at an early age. With Z. Simon, I. Moţoc, and A. Chiriac, I wrote a book that was published as *Lecture Notes in Chemistry* No. 15 by Springer Verlag [6]. The authors did not receive any royalties, but they received a few copies of this book. We had to type the manuscript on special paper sheets sent by the publisher in camera-ready format. For this purpose, we paid a professional typist and a professional person to draw figures and formulas with stencil. Any typo meant retyping/redrawing the page. After this, in order to obtain the authorization to send any manuscript abroad by mail, it had to be forwarded to a political censorship authority, and after the corresponding waiting period, it was either turned down, or returned with the permission. Imagine our desperation when on obtaining the permission, the pages of the camera-ready manuscript were returned, but having on each page a "permission granted" stamp in deep-violet color! Of course, we had to have all 178 pages retyped and redrawn again – and this took many extra months.

Dr. Dennis Rouvray visited me several times in Bucharest with his family, and we co-authored a review on chemical applications of graph theory [7] for the two-volume publication of Robin J. Wilson and Lowell W. Beineke: the first volume was a collection of chapters on selected topics in graph theory [8], and the second volume that appeared one year later contained applications of graph theory in communication networks, electrical networks, statistical mechanics, operational research, social sciences, geography, architecture, and linguistics. Seeing the conditions in Romania, he proposed to help me emigrate. I replied that I wanted do so, but only provided that my family could accompany me (otherwise, my wife would lose her job at the Polytechnic, and with our children she would hardly be able to sustain a decent existence, with us living separately for an indefinitely long period). He kindly replied that he would try to make arrangements that this topic would be raised during a soon-to-be official visit of Robin Wilson's father (Harold Wilson, the Labour Party leader and Prime Minister of Great Britain). Apparently, nothing came out of this attempt, but the communist Romanian authorities became even more displeased with me.

During my last visit at the Max-Planck-Institut für Strahlenchemie, I raised the possibility of staying in the West, and Professor Polansky graciously agreed to offer me a position. However, on contacting with discretion the German immigration authorities, he learned that I would have to ask for political asylum, that I had to live for several months in a camp for refugees, and that there was no serious hope for my family to be allowed to join me in a foreseeable time. Thus, I had no other choice but to return to Romania.

Two other events (unrelated to the anniversary, but illustrating the atmosphere) will be mentioned. The first one originated in the fact that in the Bucharest Institute of Atomic Physics (where I was in charge of a small laboratory for isotopically labeled

compounds) a larger laboratory had built their own electron spin resonance spectrometer, and needed 2,2,-diphenyl-1-picrylhydrazyl (DPPH) as a standard for the ESR spectra, so they asked us, the organic chemists, to prepare it. After having done this, I wondered about the reason for the extreme stability of this free radical, and I hypothesized that steric and electronic factors might be responsible. In order to test the first parameter, we synthesized related free radicals having only two instead of the three nitro groups of DPPH. Indeed, the 2,6-dinitro-derivative was as stable as DPPH, but the 2,4-dinitro congener could not be isolated as a crystalline compound, and decomposed slowly in solution. (Interestingly, at that time two other research groups had the same idea in USSR and Hungary, and thus three papers described similar results obtained independently and simultaneously). It was evident that the steric factors were not the main reason for the stability of DPPH, so that we had to test the electronic factors, by synthesizing other *"push-pull"* aminyls. We were successful [9], and some years later several other research groups applied this idea for stabilizing carbon free radicals: Katritzky and his coworkers in Norwich, England (now in Gainesville, Florida) prepared *"mero-stabilized"* free radicals [10], while Viehe, Merényi, Janousek in Belgium (with Stella from Marseille, France) prepared other such radicals stabilized by the *"capto-dative effect"*, citing our priority [11]. This effect had been discussed theoretically by Dewar [12], but without reference to the stable hydrazyls. In 1986, Heinz Viehe organized in Louvain-la-Neuve a NATO Advanced Research Workshop, to which I was invited. By an unexpected stroke of luck, I could attend the meeting (I had not disclosed that it was under the auspices of NATO), I gave the invited lecture, but I did not dare to have it printed in the volume. However, my name (with my home address, in order not to cause any inconvenience to my university) is there among the list of participants [13].

The second event is connected with Roald Hoffmann, who had visited Romania several times, even before he had obtained the Nobel Prize for Chemistry. We two had been friends for a long time, and twice he asked me to recommend young Romanian chemists for post-doctoral assignments with him at Cornell University. The first one was Mihai Elian, who published several important papers with Roald; the second one was Mircea Gheorghiu. Both returned to Romania after their stay in the USA. Having seen how the research situation in Romania deteriorated continuously during his successive visits, Roald Hoffmann sent during the mid-80s a detailed letter to Elena Ceauşescu in the hope that he would help our cause. He sent copies of this letter to me, to Mircea Gheorghiu, and to Mihai Elian, who after Nenitzescu's death had become the Deputy Director of the Academy's Research Institute for Organic Chemistry. Elian is a co-author of the last paper in ref. [9]. Roald had written that letter with the best intentions, but without consulting with us. We would have told him that the effort was hopeless, and that this letter would lead, on the contrary, to punitive measures against us. After about one month of dreading the worst, nothing happened and we realized that probably the letter had been stopped somewhere by those political advisors who knew that the addressee would feel insulted, and the situation was hopeless. Roald never got any reply to his well-meaning letter.

Unfortunately, the promising research of Mihai Elian was suddenly cut a few years later by a fatal heart attack. Mircea Gheorghiu teaches now at MIT, and I am a professor at the Texas A&M University in Galveston. Scientific research in Romania has not yet recovered after the disaster caused by Elena and Nicolae Ceauşescu.

Conclusion

The 30th anniversary of MATCH is an opportunity to look back and to be grateful to Professor Polansky's open-mindedness and generosity in providing to chemical graph theorists a peer-reviewed journal that published many of their papers, and to develop a close-knit group of scientists coming from different countries and fields of chemistry (inorganic, organic, physical, computational) or of mathematics. Instead of competing with each other, this group encouraged collaborations and an attitude based on the motto "let us learn from each other".

I strongly hope that this field, which has proved its importance by the numerous papers, symposia, and books during the last decades, will continue to flourish, and that the scientists will continue the tradition of openness and collaboration that has existed for many decades.

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