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Editorial

Introduction and Foreword to the Special Issue Commemorating the Thirtieth Anniversary of Eiji Osawa's C_{60} Paper

INTRODUCTION

The Guest Editor of this issue, Professor Zdenek Slanina, is well known in the field of fullerenes. He has published more than 300 original papers and 25 book chapters and reviews, including a chapter in *Reviews in Computational Chemistry*.[1] In addition, he has edited three books. Among his many recognitions, he was listed among leading authors in fullerene research in a survey published in *Angewandte Chemie, International Edition in English* (1992, **31**, 588). Also, he was listed among the 4,000 most-cited chemists in the world by the Institute of Scientific Information (Philadelphia, Pennsylvania) in 1997.

Since 1996, Dr. Slanina has held the position of Professor in the Department of Knowledge-Based Information Engineering at Toyohashi University of Technology in Japan. Before that, he was Visiting Scholar/Professor at National Chung-Cheng University in Taiwan, Republic of China, for three years. He is believed be to the first European to receive full-professor certification from both the Taiwanese and Japanese educational authorities.

Dr. Slanina's interesting journey eastward formally began in November 1985 when he went to Hokkaido University on a study leave. However, the roots of his journey can be traced back to a dark moment in modern Czech history: the Soviet Socialist military invasion of Czechoslovakia on August 21, 1968, the same day he turned 20 years old. In spite of the Soviet occupation of his country, he continued his studies and obtained a Graduate Chemist (B.A.) degree in chemistry in 1971, followed by a Rerum Naturalium Doctoris (M.A.) in 1971, both from Charles University in Prague. In 1975, the same year he was married, he was awarded the Candidatus Scientiarium (Ph.D.) degree after research in the Czechoslovak Academy of Sciences. His thesis was on semiempirical calculations of equilibrium constants. His first appointment was as research assistant at the J. Heyrovsky Institute of Physical Chemistry and Electrochemistry in Prague. His career at the institute advanced steadily, but at the same time he yearned for greater opportunity and freedom. He tried three times and failed to receive local administrative approval for study in Sweden, the United States, and Germany. It became obvious that it would be better to try to go to some remote country, at best a nonmember of NATO.

In the mid-1980s Dr. Slanina shared an interest in isomerism with Prof. Eiji Osawa at Hokkaido University in Japan. Prof. Osawa was primarily interested in isomers of large organic molecules, whereas Dr. Slanina computed various small clusters, which was the subject of a later book.[2] Dr. Slanina applied for a leave of absence and, after he waited many months, the Czechoslovakian authorities finally allowed him to go to Japan. Dr. Slanina left Prague on November 15, 1985. Although the intent was to study isomerization in Sapporo, a momentous paper was published in the November 14, 1985, issue of *Nature*.[3] This was the buckminsterfullerene paper by Kroto et al., that would lead to a Nobel Prize. Unknown to Dr. Slanina (and many others) at the time, Prof. Osawa had in 1970 proposed the C_{60} structure, and Prof. Osawa had no idea that Dr. Slanina computed small carbon clusters. The match of their interests, plus the buckminsterfullerene paper, led to a serendipitous confluence of events.

Instead of the planned study of rotational isomerism, work during Dr. Slanina's stay in Sapporo focused on computing C_{60} and C_{70}. Those large species were just on the edge of the possibilities of the supercomputers available at that time, and there were many interesting related events.[4] Fortuitously, a hidden and tricky hardware/software bug in the Hokkaido University computer system allowed an additional allotment of the CPU time, which in turn made possible the completion of a year-long computation.[5]

Still another fortuitous happenstance made possible Dr. Slanina's work in Sapporo. Whereas obtaining administrative approval on the Czechoslovak side was very difficult, obtaining approval from Japanese authorities was not straightforward either. There was a hidden rule that scholars from then Communist countries should not be allowed to use Japanese supercomputers. Every applicant for a long-term visa in Japan had to write a one-page essay on the purpose of the trip. If the word "supercomputer" was found in the essay, the application was automatically turned down, and there was no chance to reverse the negative decision. Dr. Slanina was unaware of the basically

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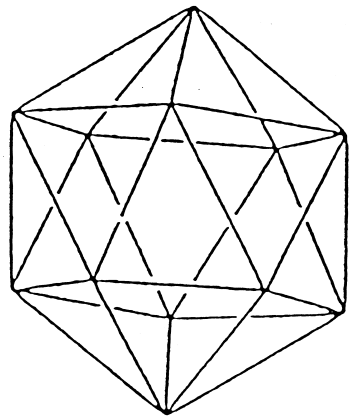
多数のベンゼン環の縮合した型のいわゆる"縮合多環式芳香族炭化水素"は典型的な平面分子である．これらの代表的なベンゼノイド芳香族が球状分子の型をとったなら超芳香族性を示さないだろうか？　たとえばサッカーの公式ボールの表面に描かれている幾何模様を思い浮かべてみよう．それは正多面体としてcubeのつぎに小さな正二十面体(eicosahedron)(*12*)の頂点を全部切り落として正五角形を出したもので，truncated eicosahedronとでも称されるべき美しい多面体である(*13*)．図ではわかりにくいところもあるので，もし手もとにサッカーボールがあれば手にとってながめていただくとはっきりするが，五角形(黒く塗ってある)の間には規則正しく六角形がうずまっている．一見これらの成分多角形はたいして曲がってもいないし，各辺はすべて同じ長さにすることができる．もしこれらの頂点を全部sp^2炭素



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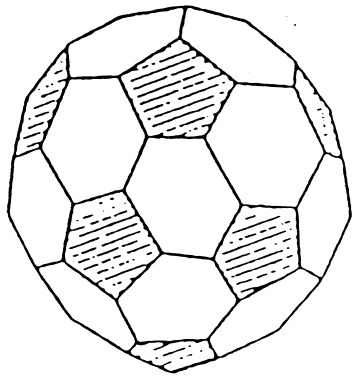

(*13*)

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Figure 1. Reproduction of Osawa's illustration of C_{60}; used with permission of Kagaku-Dojin Publishing Co., Inc.[12]

secret rule. However, he, like Enrico Clementi of IBM, believed that the term was artificial. The best computer of every era could be called a supercomputer, and with the course of time the name would shift from one machine to another. So,

Dr. Slanina did not use the word supercomputer in his visa application and got the visa!

In the late 1980s and early 1990s, Dr. Slanina held a variety of visiting scholar positions in Germany, the United States, and Belgium. Despite the collapse of the Iron Curtain in 1989 and the ensuing burgeoning of freedom in Eastern Europe, his interest lay in the east. In 1993, the year the Czech Republic was established, he went to National Chung-Cheng University in Taiwan. In 1995 he was awarded the university qualification degree by the Taiwanese Ministry of Education and became a full professor. However, for someone interested in fullerenes, Toyohashi in Japan offered an irresistible allure. Prof. Slanina points out that not only was Prof. Osawa there, but also the fertile fields in warm central Hsinchu provide a locale for growing two kinds of spheres—melons in the summer, and cabbage in the winter. Prof. Slanina jocularly reports that it seemed natural for Prof. Osawa and the people around him to study fullerenes in such a "sphere-friendly environment." Asia continues to hold a fascination for Prof. Slanina.

It was fortuitous for this journal when in April 1999 Prof. Slanina proposed organizing this special issue. As he pointed out, Prof. Eiji Osawa's work on C_{60} was one of the most successful predictions of molecular modelling. Prof. Osawa's achievement illustrates that the key to a successful design is not simply doing a computer calculation, but rather using the mind to conceive an original idea. I congratulate Prof. Eiji Osawa on the anniversary of his elegant contribution to science as well as for his many other accomplishments. Finally, I sincerely thank Prof. Slanina for bringing together the papers appearing in this celebratory issue, and I welcome the authors.

Donald B. Boyd, Ph.D.
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FOREWORD

Molecular modelling has not always been treated as an equal and productive partner with experimental science. Nevertheless, modelling can be traced back well into the 19th century, although not under this name. The start was not smooth, and for decades theoretical predictions in chemistry were not taken as seriously as those in physics. We are lucky to live in a time when it has finally come to be so. In 1874, 22-year-old J. H. van't Hoff, and soon thereafter also J. A. Le Bel, predicted tetrahedral carbon coordination. However, the reception to the new concept was pretty unfriendly.[6] One of the leading scholars of the time, H. Kolbe, wrote: ". . . A Dr. J. H. van't Hoff, of the Veterinary School at Utrecht, has no liking, apparently, for exact chemical investigation. He has considered it more comfortable to mount Pegasus [apparently borrowed from the veterinary school]. . . . The practical chemical world had little liking to these hallucinations . . ." H. Kolbe showed his disdain of theoretical modeling when he wrote, "Where . . . and since when have games been called chemical theories." The aftermath of such criticism was probably still being felt in 1901 when van't Hoff was awarded the Nobel Prize, but he received the prize for his work on osmotic pressure, whereas the tetrahedral carbon was mentioned only in the presentation speech.

Speculations and predictions in chemistry have been more welcome since World War II. This improved situation is exemplified by the congressane (diamantane) story. Congressane, which had not yet been prepared, was featured as an emblem of the XIXth International Congress of Pure and Applied Chemistry in London in the summer of 1963. Two years later, the compound was prepared[7] by P. von Ragué Schleyer et al., and yields were improved in 1970.[8] In a sense, adamantanes can be called the fullerenes of the 1960s. Moreover, adamantane and diamantane are formally just hydrogenated pseudo-fullerenes.[9]

At Princeton University, Eiji Osawa worked with Professor Schleyer for two years, doing work not only on congressane but also on another polyhedral hydrocarbon, bastardane.[10] Dr. Osawa returned to his homeland and continued to pursue his interest in cage compounds.[11] Having fresh experience that predictions and speculations are a legitimate part of chemical research, Dr. Osawa published in 1970 a proposal that a C_{60} cage in the form of a truncated icosahedron could be a stable species with interesting properties that he termed superaromaticity.[12] The original graphic is reproduced in Figure 1.

Dr. Osawa's proposal had no immediate impact on chemistry. Only since 1986 has his article been recognized as "the first known suggestion by a chemist that C_{60} might be stable."[13] The delay in recognition resulted from the proposal being published in Japanese and not being well abstracted.[14] Other early theoretical suggestions[15–19] dealing with C_{60} also had no direct experimental consequences[20–22] (with the exception of a discussion of O. L. Chapman et al. in a survey).[23] The predictions simply came too early, when chemistry was not prepared for the task and also at a time when theory could not been always trusted.

Prof. Eiji Osawa's fullerene prophecy from 1970 can be viewed as a kind of molecular modelling and also as a kind of molecular graphics. Thus, it is entirely appropriate to celebrate the 30th anniversary of his C_{60} proposal with this special issue of the *Journal of Molecular Graphics and Modelling*. I would like to thank Kagaku-Dojin Publishing Co., Inc., for permission to reproduce Figure 1. I also thank all other contributors in this issue for their kind effort and cooperation.

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