

# A history of the international group for correlation analysis in chemistry<sup>†</sup>

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**ABSTRACT:** The author has been Secretary of the International Group for Correlation Analysis in Chemistry (formerly Organic Chemistry) since it was founded in 1982. A series of conferences in the USA, which began with a Symposium on *Linear Free Energy Correlations* at Durham, NC, in 1964, eventually stimulated the development of a similar series in Europe, starting with a conference on *Correlation Analysis in Organic Chemistry* at Assisi, Italy, in 1979. This conference established a continuing organization in a provisional form and, at the second conference in Hull, UK, in 1982, this became the International Group for Correlation Analysis in Organic Chemistry. The conferences have continued ever since at intervals of between two and three years at venues in Europe or (on two occasions) in Asia, and now total nine. The Group (which dropped the 'Organic' from its title in 1991) has been an Associated Organization of IUPAC since 1990. The article describes the development of the Group as a society during twenty years and its various activities, including the conferences and a substantial Newsletter, produced at intervals of six months to a year for 24 issues. Copyright © 2003 John Wiley & Sons, Ltd.

**KEYWORDS:** correlation analysis; linear free energy relationships; chemometrics

## INTRODUCTION—THE PREHISTORY

From October 19 to 21 1964, a Symposium on *Linear Free Energy Correlations* was held at Duke University, North Carolina, under the auspices of the US Army Research Office, Durham.

I do not know whose idea it was to hold this Symposium, but the physical organic chemists on the Organizing Committee were E. Grunwald (Brandeis University), J. Hine (Georgia Institute of Technology), C. D. Ritchie (SUNY, Buffalo), and R. W. Taft (Pennsylvania State University). The mid-1960s was certainly a good time to hold such a meeting, as may be seen from the titles of the papers and the names of their authors. Many of the topics were soon the subjects of publications which became well-known as landmark contributions to linear free energy relationships (LFER). Most of the participants were from USA, but there were also quite a lot from outside North America.

The Symposium was regarded as very successful and a decision was taken to hold another in a few years time. It was eventually held in March 1968 at the new campus of

the University of California, Irvine. The title of the conference was essentially the same as that of the first: *Linear Free Energy Correlations* or perhaps ... *Relationships*. Among other contributions made, C. G. Swain presented the treatment of substituent effects that ultimately became well known as 'Swain and Lupton' and Y. Yukawa presented a development of the earlier work of Yukawa and Tsuno.

The Irvine meeting marked the beginning for me of about a dozen years of association with this series of conferences, which was the spur to getting something similar going in Europe. The third in the series was in the Spring of 1971 at Florida State University in Tallahassee. This event marked a change in the general nature of the topics included in the conferences: the title was changed to *Structure–Energy Relationships*, and the emphasis was on gas-phase reactivity and quantum mechanical treatments. LFER still played some part in the contributions. There was a small group of participants from outside the USA. The next Symposium was held in San Juan, Puerto Rico in January 1974. There was one in 1977, although I did not attend. There was also one in March 1980, at Georgia Institute of Technology, Atlanta, which I did attend. However, by that time, there had been developments in Europe: an International Conference on Correlation Analysis in Organic Chemistry had been held in Italy about six months earlier and another one was already being planned for the UK in 1982. We must now backtrack a few years in our story.

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<sup>†</sup>Dedicated to Professor Dr Marek Krygowski for his 65th birthday, in recognition of his contributions to physical organic chemistry and especially to the life of the CAIC Group.

In the early 1970s some of the participants in the American conferences from outside the USA, particularly from Europe, had begun to discuss spasmodically whether it would be worthwhile organizing a series of similar conferences at European venues. The atmosphere of the American conferences, fairly small and informal, had been attractive. It became clear, however, that a European series would probably return to the original emphasis of the American series, LFER, while not excluding gas-phase reactivity and molecular orbital treatments. At that time the term 'correlation analysis in organic chemistry' (CAOC) was coming into favour to describe the research area that had commonly been referred to as 'linear free energy relationships', and in discussing possible conferences (initially just one, of course, as a trial) this new term was often used. It also became clear that quite a few American colleagues would probably participate in European conferences which recovered something of the original emphasis of the American series.

Since the late 1950s I had travelled a great deal in Europe and North America and had built up an extensive network of contacts in physical organic chemistry, particularly in LFER. Further opportunities for making such contacts had developed with the starting of the International Conferences in Physical Organic Chemistry under the International Union of Pure and Applied Chemistry (IUPAC), the first being held at Crans-sur-Sierre in Switzerland in 1972 and the second near Leyden in The Netherlands in 1974. Indeed some were wondering whether we should try to find a home for Correlation Analysis meetings as part of the IUPAC conferences. However, there was another view that it would be difficult to create the atmosphere of a small informal meeting as part of a large meeting.

In April 1975 I went on a two-week tour of Universities and Institutes in Poland. I mentioned the idea of a European meeting on CAOC to several Polish colleagues and found that they would be keen on such a project and to hold it in Poland. Piotr Tomasik (then in Częstochowa) and Romuald Zalewski (Poznań) were particularly enthusiastic.

One physical organic chemist whom I did not meet on that trip to Poland was Dr Marek Krygowski (Warsaw), because he was then on a year's Visiting Professorship at the University of Guelph in Ontario, Canada. I already knew him by correspondence, but had never met him. However, it became possible for me to meet Krygowski at the home of Marvin and Barbara Charton in Brooklyn Heights in the first weekend in July 1975. During this time Marvin, Marek and myself spent one day visiting Professor and Mrs Hammett in their retirement community in Medford, NJ, as described in my Hammett Memorial Lecture in 1988.<sup>1</sup> Our discussions during the weekend included the possibility of a European meeting on CAOC; Marek was as keen on the idea as Marvin and I were.

A further opportunity for discussion with Piotr Tomasik occurred in early August 1975, when I was enjoying a mountaineering holiday in the High Tatra of southern Poland. Tomasik and his family were on holiday in Zakopane and he and I met for an hour or two at a convenient mountain hut. By that time Tomasik and his colleagues had agreed that they would organize an International Conference in Correlation Analysis in Organic Chemistry, probably in the summer of 1977.

For about the next two years the Polish chemists struggled to implement their intention. I have never heard anything like a full account of the problems they were trying to overcome. Some of these were no doubt connected with the Communist bureaucracy, but the factor which finally led to the collapse of the project was the appalling state of the Polish economy at that time. This made it extremely difficult to budget for the holding of an International Conference and to give potential participants, particularly those from outside Poland, any idea of the likely cost of attending. By the middle of 1977 no real progress had been achieved, although the Polish friends remained ever optimistic that this was only just around the corner. With the agreement of some of the physical organic chemists who had been consulted at an earlier stage, I wrote to Tomasik to ask him to tell me quite frankly whether there was really any hope of holding the proposed conference in the foreseeable future. The answer was in the negative and he suggested that we should enlist the help of colleagues in another country, which did not have the problems of Poland. It appeared that Tomasik already had another country in mind: Italy, where he had a very good friend in Professor G. Marino, well known as a physical organic chemist, at the University of Perugia. I wrote to Marino (whom I had met at the 2nd IUPAC Conference in 1974) and he replied that he and his colleagues would be delighted to organize a conference along the lines envisaged. And so planning began for an International Conference on Correlation Analysis in Organic Chemistry, to be organized from the University of Perugia, and to be held in nearby Assisi, from Sunday September 9 to Friday September 14 1979.

## THE EARLY DAYS—THE CONFERENCES AND THE GROUP

### Assisi 1979

The planning of the Assisi conference was almost entirely in the hands of Professor Marino and his colleagues in the Chemistry Department of the University of Perugia, particularly Sergio Clementi, as Secretary. It is probable that some of us who had been concerned with initiating the European project were asked for suggestions regarding topics and main speakers, but I have no recollections of this. The Italian colleagues obtained good sponsorship from their University, learned societies, government

agencies and industry (particularly pharmaceutical companies). Moreover, recognition by the European Federation of Chemical Societies was obtained, so that the meeting could be described as a EUCHEM Conference. There was no financial support directly arising from such recognition, but the title was important, particularly for a new venture coming, so to say, 'out of the blue'.

The later conferences are described in some detail in the Group's Newsletter, but no such records exist for the first two, and I have to rely on my memory of what happened about 24 years ago. The conference was held in the Cittadella Cristiana, a facility used for most of the year to house pilgrims to the town of St Francis. The accommodation for participants was simple but adequate (there were some grumbles!), the food was good, and the facilities for the lectures and poster presentations were well arranged. There was a good international spread of participants, both European and from further afield. The former included Otto Exner (Prague), Marek Krygowski, Marie-Françoise Ruasse (Paris), Christian Reichardt (Marburg), Svante Wold (Umeå, Sweden) and Jan Engberts (Groningen), most of whom have become firm supporters of the conferences, and also Viktor Palm (Tartu). It was a major achievement of the conference organizers, and of Palm himself, to succeed in overcoming the obstruction of the USSR bureaucracy and secure his attendance. From North America came Bob Taft, Corwin Hansch (Claremont, California), the Chartons, Alan Katritzky (Gainesville) and Jack Edward (McGill University, Montreal). From even further afield came Yuho Tsuno and Ron Topsom. The total number of participants was about ninety.

At the final session of the conference it was warmly agreed that the conference had been a great success and I was asked to arrange another at some appropriate venue in the UK in 1982. The question of a continuing organization was also discussed. The people present at Assisi seemed rather cautious about this, but it was finally agreed that a start should be made by applying to have a CAOC Subsection in the already existing Chemometrics Society. Sergio Clementi was willing to try to bring such an organization into existence and act as Secretary until the 1982 conference, including producing an occasional Newsletter.

## Hull 1982

The actual venue for CAOC II had not been decided at Assisi. When I returned to Hull I consulted my colleague Professor Norman Chapman, with whom I had been collaborating in physical organic research and writing for 23 years.<sup>2,3</sup> We held discussions with other colleagues, and decided that we could commit ourselves to organizing CAOC II, using the conference facilities of the University of Hull Residences at The Lawns, provided we could secure the support of the Royal Society of Chem-

istry, Perkin Division. Geoffrey Collier agreed to act as Secretary.

The support of the RSC and in particular of its Conference Office headed by Dr John F. Gibson was crucial. We did raise some money from local industry, but we were effectively given a blank cheque of financial support by the RSC, on the understanding of course that we behaved prudently. The finances of the conference, applications to attend, and printing were handled by the RSC Conference Office, while we in Hull put the scientific and social programme together and dealt with domestic matters regarding accommodation, meals, etc. As in the case of the Assisi conference, we also obtained EUCHEM recognition, so that the official title of CAOC II was the Second EUCHEM Conference on Correlation Analysis in Organic Chemistry. It came to be scheduled as one of the 'July conferences' of the RSC for 1982: Sunday July 18 to Friday July 23.

The year 1980 was an important year in the development of CAOC II. As already mentioned, I attended the sixth of the American Meetings (in Atlanta) in March. In April I had a brief visit to Poland, to participate in a Joint Polish-Czechoslovak Symposium on aspects of thermodynamics in chemistry at Kazimierz-Dolny (south-east of Warsaw), at which there were a small number of west European visitors. Both these events provided good opportunities for contact with physical organic chemists and I met Marek Krygowski for the first time on Polish soil. The Polish event also provided me with an opportunity to hold a kind of meeting of the International Committee of CAOC II, involving some actual members of the Committee (Krygowski, Marino, and Reichardt) and other potential participants.

The year 1981 unexpectedly provided another opportunity of meeting Marek Krygowski, when he was spending some weeks in early summer with Christian Laurence and colleagues at the University of Nantes. By the beginning of October 1981 the financial problems of many Universities, including Hull, under the Thatcher government were beginning to cast a shadow over academic life in the UK. Early retirement schemes for senior members of staff began to be discussed. There was no compulsion, but various inducements to volunteer were on offer. By early 1982 it had become clear that I might well find it more pleasant to spend the last quarter of my academic life 'doing my own thing', than by remaining in post. By March my early retirement had been agreed by the University for September 30 1982. If I had not early retired when I did, I would not have been able to undertake the organization of the correlation analysis group.

In early July 1982, a potentially serious problem for the participants at CAOC II appeared: a railway strike was threatened. By the time we had reached just a few days before the conference, the strike was in progress. Many of the participants were intending to travel to Hull by train. A major operation to enable our participants to reach us from all over the world in spite of the strike was mounted.

In one way or another all the participants, around ninety in number, arrived at The Lawns site by about 9.00 pm. The strike was settled during the next day or two.

My main (easily accessible) record of CAOC II is a copy of the book of Abstracts. Since there was no Newsletter account of CAOC II, we will list the nine Plenary Lectures here, to give the general flavour of the conference: 'Correlation Analysis—Retrospect', N. B. Chapman (Hull); 'An Overview of the Two-Parameter Approach to the Quantitative Description of Electrical Effects', M. Charton (Brooklyn); 'Theoretical Estimation of Steric Effects on Chemical Reactivity', D. F. DeTar (Tallahassee); 'Solvent Effects and Effects of Substituent Solvation', R. W. Taft (Irvine); 'Solvent Effects in Organic Chemistry: an Approach through Multidimensional Statistics', M. Chastrette (Lyon); 'Applications and Limitations of Correlation Analysis in the Field of Polymerization Reactions', G. Heublein (Jena); 'Substituent Effects and Molecular Geometry', A. Domenicano (Rome); 'Concerning the  $N_+$  Correlation', P. O. I. Virtanen (Oulu); 'Correlation Analysis—Prospect', O. Exner (Prague). There were also 21 oral contributed papers and 49 posters.

The plenary lectures and also the contributed papers contained much that may be described as studies involving LFER, but the developing alternative or complementary treatments were not neglected, including the use of sophisticated statistical methods (chemometrics) and quantum mechanical calculations, *ab initio* or otherwise. The main chemical reactivity areas of substituent, solvent and reagent effects, and the correlation analysis of spectroscopic frequencies or intensities were certainly well covered, along with applications involving crystallographic data. Gas phase reactivity was not very evident, nor was the biological activity of organic compounds (QSAR).

At a concluding business meeting, Sergio Clementi reported that he had duly established a continuing organization as the CAOC Subsection of the Chemometrics Society, had recruited members and compiled a membership list, and had produced two Newsletters. He had, however, begun to be somewhat disillusioned, because he felt there had been little support from most of those who were supposed to be members. If such a group were to be useful, much more effort by the Secretary would be needed and Clementi would not be able to do this. The meeting felt that the connection with the Chemometrics Society had probably been a mistake and that an independent Correlation Analysis Group would be more attractive to most physical organic chemists. I agreed to reorganize the Subsection under the name of International Group for Correlation Analysis in Organic Chemistry and to see what could be accomplished by the time of the next conference. It was now assumed that there would be such a conference and a tentative offer to host it in 1985 was conveyed from the physical organic chemists at Louvain-la-Neuve. It was also suggested that, in the meantime, the attempt to keep in touch with members of

the new Group through a Newsletter should be pursued. Geoffrey Collier agreed to act as Treasurer.

### The CAOC group 1982–1985

During 1982–1983 Clementi and I took various actions to wind up the CAOC Subsection of the Chemometrics Society and to transfer those of its members who so desired to the new Group. A membership form was sent to Subsection members as part of a final Newsletter, to the participants at CAOC II and to some other physical organic chemists who might be interested. The response was patchy, and I decided also to regard as members various people whom I knew to be interested in CAOC, but who had neglected to reply. This action on my part increased the membership to approaching 190. No-one who was forcibly recruited in this way subsequently raised any objection when their names and addresses were included in the first membership booklet, which was circulated with the first Newsletter at the end of 1983.

The final action of Clementi with regard to the CAOC Subsection was to transfer their bank balance to the CAOC Group, and this made a good initial deposit in our account. A request for financial support had accompanied the membership forms. From the start it was made clear that there was no question of imposing a subscription, but we would request a minimum financial contribution from time to time, and ask members to be as generous as possible. The point was that, at that time, there were a considerable number of countries from which it was almost impossible for private individuals to send money abroad. These countries included the USSR and the Soviet satellites of eastern Europe, and the developing countries. We already had quite a lot of members in these countries, and expected to recruit many more. To impose a subscription would effectively render their membership impossible. This matter had been raised, discussed, and settled at the business meeting in Hull. The financial basis of the Group has remained the same ever since, although the number of countries with foreign exchange difficulties is now very much smaller. The first request was for a minimum of about £3 or its equivalent and it was implied that further help would not be solicited for several years. A triennial arrangement of our finances, corresponding to the usual interval between our conferences, was thus effectively established at an early stage.

The importance of having a worthwhile Newsletter had been emphasized in the discussions at CAOC II, and I produced the first one with a date of December 1983. This was entitled Newsletter No. 1 (New Series), to imply recognition of what Clementi had done in producing three issues for the CAOC Subsection. It had 24 A5 pages. Various items in Newsletter No. 1 (NS) were of types which have continued in many of the later issues. The first item was 'From the Secretary' and was particularly

devoted to the setting up of a 'Working-Group on Goodness of Fit'. Other items were two pieces (by me and by T. W. Bentley) about the recently published work of C. G. Swain on substituent and solvent effects, and the initial reactions of the physical organic community to this; the announcement of a new journal *Quantitative Structure-Activity Relationships in Pharmacology, Chemistry, and Biology*, and three reports on conferences in physical organic chemistry: the Seventh Conference on Structure-Energy Relationships, Monterey, California; Selectivity, Reactivity, and Structure in Organic Reactions, Maynooth, Dublin; and an ACS Symposium in Honour of Louis Hammett, Washington, DC.

Publishing reports on 'other conferences' in physical organic chemistry became a frequent feature of the Newsletter. An item 'News from Members' had contributions from about fifteen members distributed world-wide: Europe, USA, North Africa, Asia, Australasia. 'Some Recent References', occupying about  $3\frac{1}{2}$  pages, was the first of such items, which have appeared in almost every issue of the Newsletter.

Newsletter No. 2 (NS), December 1984, contained information about CAOC III, which had acquired an expanded title as the Third International Conference on Correlation Analysis in Organic and Biological Chemistry. The organizers at the Catholic University of Louvain campus at Louvain-la-Neuve, Belgium, had chosen to give CAOC III a biological emphasis. A First Circular was enclosed with the Newsletter. The Secretary's piece in NL 2, 12.84<sup>4</sup> reported membership approaching 200 and suggested a slightly larger minimum contribution of £4. The sending of a greetings telegram to Louis Hammett on his 90th birthday and of a telex message to Bob Taft on his 60th were also reported. The state of the Swain controversy was updated and a report and other material from the Working group on Goodness of Fit were presented. There was an account of the Seventh IUPAC Conference on Physical Organic Chemistry by Christian Reichardt, the first of many such reports. Special reports on 'A Polish Meeting on CAOC' (Marek Krygowski) and 'Some News of CAOC in Czechoslovakia and Elsewhere' (Otto Exner) also appeared. NL 2 had 28 A5 pages, and room was found for 2 pages of 'News from Members' and  $5\frac{1}{2}$  pages of 'Some Recent References'. The Secretary announced that he expected to be in India for about five weeks from mid-February 1985 (see Section on Other organizational matters, below).

### Louvain-la-Neuve 1985

This was held from Sunday July 14 to Friday July 19 1985. An account of it appeared in NL 3, 12.85. There were about one hundred participants, nearly forty of whom were already members of the CAOC Group and several more joined during the meeting. EUCHEM recognition had been obtained.

Professor Paul van Brandt and his colleagues introduced two new features into the Conference. The first, as mentioned already, was an emphasis on biological aspects, in five of the ten plenary lectures. The second was to have all the contributed papers (about 50) as posters. This was intended to give a more relaxed atmosphere, with plenty of time for discussion. The experiment was interesting and worth making, and up to a point was successful. The posters were in position throughout the conference, divided into three groups for three poster sessions. The distinction between the three groups became blurred, however, and by the last poster session it was clear that the possibilities of discussion had been exhausted. None of our later conferences has followed this pattern, or has made the attempt to secure a biological emphasis. In fact the emphasis was not taken up in the contributed papers, most of these being about the usual concerns of CAOC at that time.

At the Triennial Business Meeting summary accounts for July 1982 to June 30 1985 were presented (the closing balance was reasonably healthy), and it was recommended that the the Newsletter should be produced twice a year, if practicable. Shorter and Collier agreed to continue as Officers until the next Conference, but it was thought that the time had come to have an International Committee as well as Officers. The following membership was suggested on a continental/regional basis: North America: M. Charton; Central and South America: J. Miller; Western Europe: Chr. Reichardt; Eastern Europe: T. M. Krygowski; Middle East and Africa: A. M. G. Nassar; Western Asia (particularly Indian sub-continent): P. A. Nadar; Eastern Asia: T. Hanafusa; Australia and New Zealand: R. D. Topsom. Marvin Charton agreed to act also as collector for financial contributions from members in the USA.

It was accepted that the CAOC Group had effectively become responsible for ensuring the continuation of the series of conferences, hitherto regarded as self-perpetuating. The meeting therefore dealt with the two invitations that had been received for CAOC IV, from Poland and Czechoslovakia. The Polish invitation had been received first and details were given by Krygowski, Tomasik and Zalewski. This was accepted provisionally, subject to practicalities, and the Czechoslovakian invitation was to be held in reserve.

The conference in 1985 marked the end of the first period in the history of the CAOC Conferences and of the CAOC Group, with its associated Newsletter. The general pattern of the organization and its activities was now well established and has continued largely to the present day, with some modifications and innovations. For the rest of this article, the 'blow by blow' form of account will be abandoned and material will be arranged according to topics. We will deal with the Newsletter as it has developed through its 24 issues; also with the general organization of the Group and its various activities, including the later conferences. Each conference will merit an

outline account, although the main record of the Group in this respect will have to reside in the copies of the Newsletter which are archived in the Royal Society of Chemistry Library in Burlington House, London.

## THE NEWSLETTER

An account of NL 1 and NL 2 has already been given above. After these the front cover was redesigned to include the names of the International Committee, but thereafter has remained essentially unchanged, except when the Group became an Associated Organization of IUPAC and when the Group changed its name to International Group for Correlation Analysis in Chemistry. The overall format and appearance have remained fairly constant: an A5 booklet reproduced from typed copy by offset, with the number of pages between 20 and 32, and with a tinted cover.

From 1985 I did my best to produce two issues per year, but the convenient target proved to be five issues between conferences. This was achieved fairly well up to 1994 (CAIC VI). After CAIC VI the cost of producing and distributing five issues over the course of three years became more than our finances could bear, and there was slippage towards annual issues. To compensate to some extent, most of the issues now contained 32 pages.

We must now say something about the general content of the Newsletters, apart from items directly generated by the activities of the Group (these will be more appropriately covered below in later sections). From the start I made a point of providing information about 'other conferences' involving physical organic chemistry, either by way of advance publicity or of reports afterwards. Perhaps the most important linkage was with the IUPAC conferences (ICPOC), with material often provided by Christian Reichardt. We covered ICPOC 7 to 13 comprehensively.

'Some Recent References' has been featured in most issues. The monitoring of recent work by members has also been carried out under other headings related to particular countries, institutions or individuals. We have frequently noted the appearance of new journals or new books (sometimes reviewing the latter) which may be of interest to our members.

Under the general category of news from/of members, we have reported awards and honours of various kinds to our members and events such as 60/65/70/75th birthdays. We had a special piece about the part played by our member Roger Taylor (Sussex) in the isolation, separation and characterization of the fullerenes C<sub>60</sub> and C<sub>70</sub>. Sometimes we have had to report the impact of world events on some of our members, such as the wars in the Balkans or Middle East. Sadly, it has fallen to us to record the deaths of some of our members or of other chemists well known to many of our members.

The Newsletter arrangements began to break down after the appearance of NL 23, 01.00. A year later the available finance was insufficient to produce and distribute a 28- or 32-page booklet. The best that could be done was an 8-page booklet with a condensed format as NL 24, 01.01. By early 2002 enough money was again available to produce and distribute an issue more or less along the former lines, but for various reasons this has been delayed.

## THE DEVELOPMENT OF THE CAOC GROUP FROM 1985 ONWARDS

### Formal relations with IUPAC

At CAOC IV in Poznań in 1988 it was suggested that we should seek to enter into a more formal relationship with IUPAC, informal contacts with the Physical Organic Commission of IUPAC having been developing for some time (see Section on relations with other bodies, below). On inquiry we found that the CAOC Group could apply to be an Associated Organization of IUPAC, which we duly did, and our application was finally approved at the meeting of the IUPAC Council in August 1989. It was hoped that the status would enhance our standing and perhaps make it easier for colleagues in certain countries to be members.

### The name of the group

The NL 12, 10.90 carried an item: 'Shall we change our name?' This reported a round-table discussion at Chemometrics II, the Second Czechoslovak Chemometrics Conference with International Participation held at Brno in September 1990, which was attended by about thirty of our members. In the eight years of the Group's existence there had always been the problem that International Group for Correlation Analysis in Organic Chemistry did not properly convey the breadth of interest of the membership, particularly with regard to QSAR and to certain parts of inorganic chemistry. Some years earlier we had discussed the possibility of adding Biological Activity, but it was then felt that this would be going too far. The discussion at Brno indicated that we should again try to find a title which would give a clearer impression of the scope of the Group. The simplest suggestion was that we should drop the 'Organic', and call ourselves simply International Group for Correlation Analysis in Chemistry, cf. the Chapman–Shorter monograph of 1978.<sup>3</sup> It was suggested that there should be further discussion at CAOC V in Paris in July 1991. The discussion in Paris led to the above suggestion being adopted, with the additional point that our abbreviated name should be CAIC Group rather than CAC, the 'I' standing for the 'in'. It followed that the next conference would be CAIC VI.

## Other organizational matters

There have been some changes in the International Committee: Minoru Hirota (Yokohama) replaced T. Hanafusa in 1992; W. Adcock (Adelaide) replaced Ron Topsom in 1994. Geoffrey Collier resigned as Treasurer with effect from the Triennial Business Meeting at CAIC VI in Prague in 1994, suggesting that the office could be combined with that of Secretary. I was, however, not happy to be the sole Officer and it was agreed to institute the new position of Chairman. Otto Exner agreed to fill this position.

The essential financial basis of the Group has continued as it was at the start (see Section on The CAOC group 1982–1985, above). The suggested minimum contribution to cover three years rose in stages from £3 initially in 1982 to £15 by 1994, corresponding to increase in operating costs, but the continued existence of the Group in a financially viable state has always depended very much on the generosity of a relatively few devoted members.

One of the most major changes in the organization of the Group has been the founding of its Indian Chapter. In early 1985 the Secretary spent about five weeks in India, sponsored by the Royal Society and the Indian National Science Academy (see NL 4, 06.86). From February 27 to March 1 there was a National Seminar on Linear Free Energy Relationships (Correlation Analysis) at Anna University, Madras, organized by Professor P. Ananthakrishna Nadar and his colleagues in the Chemistry Department (see NL 3). This occasion and my tour enabled me to meet a large number of Indian physical organic chemists, and to recruit many new members to the CAOC Group. Almost ten years later some of the Indian members decided to form an Indian Chapter of the Group, which would conduct various activities of its own. The key figure in this development was P. A. Nadar (by that time of Annamalai University), member of our International Committee, who became Secretary of the Chapter, with N. Balasubramanian (Bishop Heber College, Tiruchirappalli) as Treasurer. I went out to India for the Inauguration of the Chapter early in 1995, which was held in a National Seminar on Correlation Analysis in Chemistry from January 20 to 22 (NL 19, 10.95). In the last seven years the Chapter has organized various activities of its own, including an annual symposium on Students' Projects and was responsible for CAIC VIII in Chennai (Madras) in January 1999 (NL 23, 01.00).

Something should be said briefly about the growth of the membership of the Group, of which Table 1 may give an approximate idea. The sharp rise between December 1984 and July 1985 was due to recruiting in India. The decline in recent years has been due to the elimination of those whose interest in the Group has been in doubt for a long time, as well as to the normal occurrences of resignation and death. Throughout the existence of the

**Table 1.** Growth in membership of the group

Year	Month	Membership	Countries
1983	December	190	?
1984	December	≈200	?
1985	July	240	41
1988	July	270	43
1991	January	300	>40
1994	April	323	47
1995	July	338	48
2000	March	308	48
2003	February	≈300	48

Group it has never been financially possible to reprint the membership List for distribution to members more than once in about three years.

## Various activities and relations with other bodies

It has already been mentioned that in the first year of the CAOC Group's existence there was a Working group on Goodness of Fit (NL 1 and NL 2). This was chaired by Marvin Charton, and the other members were Clementi, Ehrenson, Exner and Wold. Their report was published to members of the Group in NL 2 and more widely in the QSAR Journal.<sup>5</sup>

At CAOC IV in Poznań in 1988, a Working group on 'Minimal Standards for Reporting Results of Principal Component Analysis' applied to quantitative structure–property (–activity) relationships was set up, under the chairmanship of J.-F. Gal (Nice). The membership was selected by the Chairman as follows: P.-C. Maria (Nice), M. Chastrette (Lyon), J. T. Edward (Montreal), O. Exner (Prague), U. L. Haldna (Tallinn), S. Wold (Umeå), and R. I. Zalewski (Poznań) (NL 9, 04.89). Their report was published in NL 11, 04.90.

In 1987 Paul Müller, as Chairman of the IUPAC Commission on Physical Organic Chemistry, wrote to the CAOC Group about possible collaboration between the Commission and the Group on a compilation and critical evaluation of structure–reactivity parameters (NL 7, 12.87). This was the beginning of a major undertaking. Participants at CAOC IV expressed interest in such a project. The Commission meeting at ICPOC 9 in Regensburg (August 1988) set up a Working Party under the chairmanship of Y. Takeuchi (Tokyo), with P. van Brandt (Louvain-la-Neuve) and Z. Rappoport (Jerusalem), sitting as members of the Commission, the other appointed members being Charton, Exner and Shorter. The membership was thus composed 100% of our members. Preliminary work of various kinds was done during 1988–1989 and final approval of the project by the IUPAC Organic Chemistry Division was given at a IUPAC Assembly in August 1989. At the same meeting I was appointed a Titular Member of the Commission for Physical Organic Chemistry. I held this position from 1990 to 1997 and during this period attended all the

Commission meetings. This enabled me to take a leading role in the project, which led ultimately to two Technical Reports in *Pure and Applied Chemistry*. The first was on 'Values of  $\sigma_m$  and  $\sigma_p$  Based on the Ionization of Substituted Benzoic Acids in Water at 25 °C';<sup>6</sup> the second on the extension of the classical Hammett scale by using data for the ionization of substituted benzoic acids in aqueous organic solvents.<sup>7</sup> Both these reports were reprinted in the *Australian Journal of Chemistry*.<sup>8,9</sup> A special booklet of the first report was prepared for members of the Group.

The Czechoslovak Chemometrics II conference has already been mentioned in connection with the change of the Group's name. There has been quite close cooperation between us and these conferences in Brno. Chemometrics II included a Microsymposium on Correlation Analysis in Organic Chemistry dedicated to Otto Exner for his 65th birthday. There was quite a good presence of our members at Chemometrics III (1993) and IV (1996), but no formal cooperation. This was introduced again for Chemometrics V (1999). We were responsible for some of the programme, but regrettably rather few of our members were present.

Around 1994 the Group was involved in Viktor Palm's attempt to restart *Organic Reactivity (Tartu)*, which had ceased publication in 1991 for financial reasons (see NL 17, 04.94). It was agreed that the revived journal should be described as 'published in association with IGCAIC', but the Group could not accept any financial responsibility (see NL 18, 12.94). A few issues appeared and the journal published material from Prague (1994) and Fukuoka (1996), but it then proved to be non-viable.

## THE CONFERENCES FROM 1988 ONWARDS

### Poznań 1988

The CAOC IV conference (July 17 to 23 1988) was subtitled *Hammett Memorial Symposium*, in honour of Louis Hammett (1894–1987) (see NL 8). There were some 70 participants, of whom about one-half came from Poland and the rest from 15 other countries. The previous meetings had all been EUCHEM conferences, but this was not then possible for a conference in Poland. However, CAOC IV also conformed essentially to the EUCHEM format. The venue was a conference hotel, very pleasantly situated on the edge of Citadel Park, not far from down-town Poznań. The organizers were R. I. Zalewski, T. M. Krygowski, and Z. Urbaniak. The eleven main lectures and eleven other oral contributions were all given by special invitation; there were also about forty posters, presented in three sessions. There was an additional session for a 'free discussion' of the posters as a whole, with Topsom and Reichardt as Moderators. The final session of the conference was a 'Round-table discussion on general problems of LFER and on application

of correlation analysis', with Charton, Exner and Shorter as Moderators.

The topics covered were, in principle, all those usually considered as part of CAOC, notably substituent and solvent effects, both on chemical reactivity and on physical properties (mainly spectra of various kinds). Biological activity (QSAR) was also a possible topic, but in the event received only slight attention. The methods of correlation analysis used for data treatment were commonly those of linear and multiple regression, but there was also substantial interest in chemometric techniques. Some contributions involved the role, in relation to correlation analysis, of other approaches such as quantum chemical calculations and topology.

The conference was extended by the occurrence of the Polish National Day, July 22, in the middle. Our conference in Poland was really ten years later than it should have been (see Introduction). It was held at the time of regime change in the USSR and its satellites in Eastern Europe. The organizers still had plenty of difficulties to deal with, but thankfully they were able to overcome the more serious of these. Any residual inconvenience was more than compensated by the warm Polish welcome and hospitality.

It has already been mentioned that CAOC IV was fruitful in generating new initiatives (see Sections above on relations with IUPAC and with other bodies). The conference was also fruitful in promoting publication. The main lectures were published in *Progress in Physical Organic Chemistry*, volumes 17 and 18. The book *Similarity Models in Organic Chemistry, Biochemistry, and Related Fields* was largely planned during the conference.<sup>10</sup>

### Paris 1991

There were about 120 participants at CAOC V (June 30 to July 5) from some 20 countries (see NL 13). Naturally the largest group was from France, with good attendance also from neighbouring countries. In the new international climate, colleagues from eastern Europe took advantage of their new freedom to travel and there was good representation in particular from Poland and Czechoslovakia. Unlike previous CAOC meetings in western Europe, this was not a EUCHEM conference, but the EUCHEM format was broadly followed. The national sponsors were CNRS, SFC Division de Chimie Physique, and Université de Paris 7. The organizers were led by Jean-Pierre Doucet and Annick Panaye, who had obtained financial support from about 15 organizations and firms. The working part of the conference was held in the Cité Universitaire, with most participants living in nearby hotels.

The scientific sessions were arranged on a day basis to cover the main themes of the conference as follows: Chemometrics, Solvent Effects and Gas Phase,



Organized Media, Substituent Effects and Similarity, Computer Graphics and QSAR. There were 12 main lectures, 24 shorter oral contributions and about 60 posters, covering a wide range of the concerns of correlation analysis. Once again it was clear that, while there was increasing interest in modern statistical techniques, many chemists still found discussions involving linear or multiple regression to be eminently worthwhile.

The conference was the occasion for honouring F. G. Bordwell, J.-E. Dubois, O. Exner, and R. W. Taft for 'their pioneering and continuous outstanding contributions in the fields of physical organic chemistry' and presenting them with bronze medals. The Secretary of the Group also received a bronze medal.

The July/August 1992 number of the *Journal de Chimie Physique* was devoted to the proceedings of CAOC V, with reproduction of the full texts of nearly all the main lectures and shorter oral contributions.

### Prague 1994

An invitation to Prague had first been extended for CAOC IV in 1988, so it was good that we were able at last to accept for CAIC VI (September 4 to 9; see NL 18). There were about 80 participants from some twenty countries. Naturally the largest group was from the Czech Republic, along with a small contingent from Slovakia. The Japanese representation was the strongest ever and, for the first time, there was a group from Korea. Twenty of the participants had been at ICPOC 12 in Padova the previous week. The core of the organization was provided by Miroslav Ludwig, Oldrich Pytela and their colleagues from the University of Pardubice, which provided support in various ways, and several firms helped financially. In the current period of drastic changes in the Czech Republic, the financial arrangements were not without their problems, but worked out all right in the end. The enormous Hotel Pyramida provided an excellent environment for living and working. There were 14 main lectures, over 20 other oral contributions, and over 40 posters. The various sessions through the week covered successively the themes: Opening Lectures, Substituent Effects, Studies of Reaction Mechanisms, Solvent Effects, and Theoretical and Quantum Chemistry.

By courtesy of Viktor Palm, most of the papers in issue No. 1 of Volume 29 of the revived *Organic Reactivity (Tartu)* were based on communications given at CAIC VI (see Section on Various activities and relations with other bodies, above).

### Fukuoka 1996

Around 1992 various non-European members of the Group asked me 'When is the Group going to meet outside Europe?' This matter was brought to a head in

Prague by a proposal from Japanese members through Minoru Hirota to organize CAIC VII in Fukuoka, Kyushu from August 31 to September 5, to follow ICPOC 13, which would be held in Korea the previous week. The invitation was warmly accepted, although it meant a departure from our normal interval of three years between meetings.

There were about 150 participants at CAIC VII, making it our largest meeting to date (see NL 20). Naturally the colleagues from Japan were easily the largest group, but 22 other countries were represented. The good representation from all over the world was very largely made possible by the generous funding of travelling and other expenses of many participants by the conference organizers. Minoru Hirota and Shinjiro Kobayashi and their colleagues had worked hard to raise much financial support from many firms and other organizations.

We were accommodated in several very nice hotels in downtown Fukuoka, within a short walk of ACROS Fukuoka convention centre (ACROS = Asian Cross-Roads Over the Sea). The scientific sessions were fairly intensive, occupying almost four and a half long working days. There were nine main lectures, 27 invited oral contributions, 12 short oral communications and about 50 posters.

As was the case for Prague, versions of many of the papers appeared in *Organic Reactivity (Tartu)*, courtesy of Viktor Palm.

### Chennai (Madras) 1999

The venue for CAIC VIII, as for CAIC VII, arose from the desire to make the Group less Europe-centred; an invitation to South India from the Indian Chapter (see Section on other organizational matters, above) was conveyed at Fukuoka by P. A. Nadar and accepted with enthusiasm. The dates January 10 to 14 were chosen to fall in the cooler season (see NL 23). There were about one hundred participants, of whom about one-quarter came from outside India, eleven countries being represented. Most of the overseas participants stayed at the YWCA International Guest House, which provided simple but nice accommodation and meals, with staff who were extremely helpful and courteous in providing for our needs. Many of us had not visited India previously and thus appreciated advice about sight-seeing, shopping, renting cars + drivers, etc. Attendance from outside India was greatly enhanced by generous provision of free registration, accommodation and meals for many of the overseas visitors. Financial support was provided by Annamalai University, the University Grants Commission (New Delhi), Amrutanjan Ltd. (Chennai), and the Tamil Nadu Council for Science and Technology, but there were financial problems. The main work of organization was done by Professor Nadar, together with Dr N. Balasubramaniam, Dr K. S. Rangappa (Mysore

University), and Dr V. Balasubramanian (Presidency College, Chennai).

The conference sessions were held in the Central Leather Research Institute (CLRI). The sessions occupied almost three and a half working days, and included eight main lectures, 11 invited oral contributions, and 20 short oral contributions. There were almost 50 posters, displayed in a single session.

The conference certainly achieved one of its main aims in fostering closer personal contact between the members of the Indian Chapter and the wider membership of the Group. As had been hoped, several of the overseas visitors took the opportunity of visiting various universities, colleges and institutes.

### Borówno (2001)

It is unfortunate that no issue of the Newsletter has appeared since this conference took place, although it is hoped that this in due course may be remedied (see Section on The Newsletter, above). An invitation to visit Poland again was conveyed by T. M. Krygowski and R. Gawinecki at CAIC VIII, with the implication that the venue would be near Bydgoszcz in north-western Poland. The dates of CAIC IX were ultimately fixed at September 9 to 13 2001 and a venue was found in a holiday camp at Borówno, near Bydgoszcz. The organization of the conference encountered considerable difficulties and in the outcome was the smallest we have held. There were just over 40 scientific participants. Before we were half-way through, our proceedings were overshadowed by the events of '9.11'.

There were nine invited lectures, about 20 short oral communications and 20 posters. There were two Round Table Discussions: one on Past, Present, and Future of Correlation Analysis in Chemistry, chaired by J. Shorter and E. Humeres; the other on Solvent Effects: Past, Present, and Future, chaired by Chr. Reichardt. During the meeting various awards of the Polish Chemical Society were presented to J. Shorter, Chr. Reichardt, T. M. Krygowski, and M. Cyrański.

## CONCLUDING REMARKS

I am clearly not the person to try to present an objective assessment of what the Group has accomplished during twenty years, since I have been too closely involved in its development and activities. At the very least, however, it may be claimed that the Group has been an important factor in encouraging international cooperation in a key area of physical organic chemistry, and has helped to ensure that most of the leading workers in the field have become personally acquainted and often good friends. This has sometimes happened in spite of considerable disagreements in scientific matters. Over the past few years, the topics with which correlation analysis is concerned have been changing greatly as new methods of investigation and interpretation have become important. We are also increasingly aware that our community is getting rather elderly and that young people are not joining us in sufficient numbers. The time has come when we should reassess the purposes and scope of the Group. A start was made on this in Borówno in 2001. Hopefully further progress will be made as we approach CAIC X, to be held in Pusan, Korea in August 2004 and in that conference itself.

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