

INTERNATIONAL ACADEMY OF
QUANTUM MOLECULAR SCIENCE



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50 Years 1967 - 2017

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PREFACE

The booklet "50 Years of International Academy of Quantum Molecular Science" charts a condensed version of the history of quantum chemistry in the last half century. In 1967, the five founding fathers of the IAQMS (Raymond Daudel, Per-Olov Löwdin, Robert Parr, John A. Pople, and Bernard Pullman) and a few others were convinced that quantum theory held the key to true understanding and prediction of chemical structures, properties, and reactions. To most practicing chemists of the day, they appeared to be unrealistic dreamers and visionaries.

How right were those few!

This booklet, assembled with painstaking care by Sigrid Peyerimhoff and her colleagues, will guide the reader through five decades of breathtaking developments.

January 2017

Josef Michl
President, IAQMS

PREFACE 2017

The International Academy of Quantum Molecular Science was founded in Menton (France) in 1967. For its 50th anniversary it was decided to update the booklet

”International Academy of Quantum Molecular Science –
Academie Internationale des Sciences Moléculaires quantiques
40 Years 1967 – 2007”,

written by Sigrid Peyerimhoff and Nicholas Handy in 2008.

The original outlay of the booklet was maintained. Minor changes were made in the existing text. The chapter “The years 2007 – 2017” has been added. The various lists (Bureau, members, medal winners) have been updated. The Abstracts of the meetings 2007 – 2017 and the outline of the Congresses held during this time have been added in the format given in the original booklet.

My thanks go to Jean-Marie André for writing part of the Chapter 2.4 and to Kimihiko Hirao for the histograms. Jens Meikelburger was essential for the technical support.

It is hoped that this new edition gives some insight into the life and the achievements of this Academy over the past 50 years.

January 2017

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PREFACE 2008

The International Academy of Quantum Molecular Science was founded in Menton (France) in 1967. Its members are chosen among the scientists of all countries who have distinguished themselves by the value of their scientific work, their role as pioneer or leader of a school and have most contributed to the advancement of quantum molecular sciences. The Academy provides a forum for international contact and collaboration and a periodical evaluation of the main developments, advances and promising directions of research in the broad field of the application of quantum mechanics to the study of material sciences.

When this Academy celebrated its 40th anniversary in 2007, we decided to have a look back at the origin of this Academy and the situation of the field of Quantum Molecular Science at that time. We then follow the Academy's growth and impact on the development on the entire field up to the present time in which many fields of chemistry, parts of physics and even life sciences are no longer conceivable without resorting to quantum molecular science.

The first part sets the stage for the foundation of the Academy, describes its goals and its work over the years. The second part shows the details of the work, *i.e.* lists the present and deceased members, the Abstracts of the meetings over the past 40 years, provides the list of the winners of the Annual Medal and points out important aspects of the International Congresses of Quantum Chemistry.

We hope that both parts give a realistic picture of the Academy's life within the past 40 years.

March 2008.

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2 HISTORICAL REMARKS

Sigrid D. Peyerimhoff

2.1 The State of Quantum Molecular Science

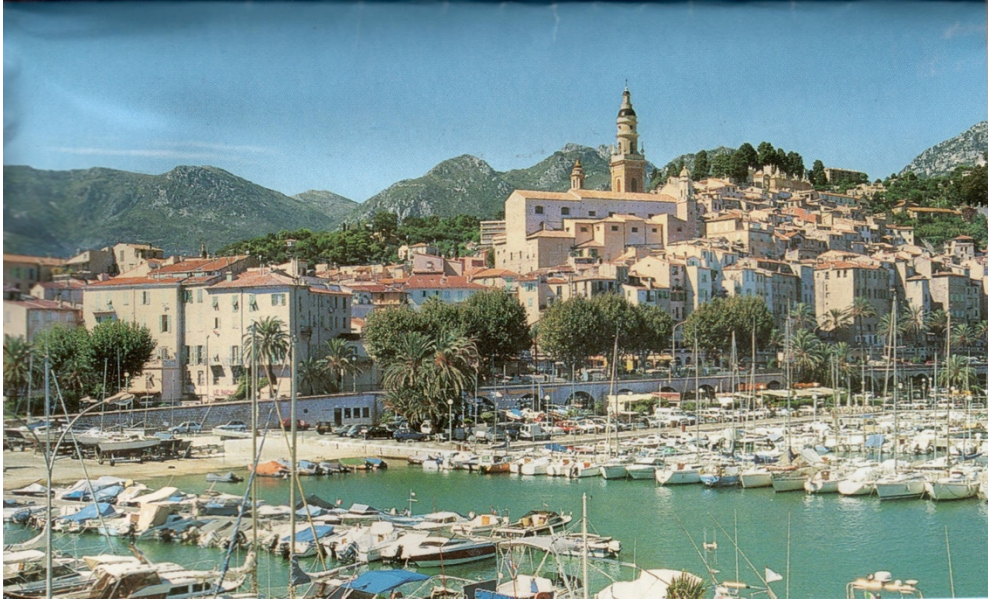
In the early years of quantum molecular science the situation is best described by the well-known dictum of Paul Dirac, Nobel Prize winning physicist at Cambridge: “The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation”(1).

Indeed, approximate methods were quickly designed by scientists in various countries. What Dirac did not – and perhaps could not – foresee was the development of *programmable* computers which lead to a major breakthrough in the entire field. The first such programmable machine was designed in Germany shortly before and during World War II; further computer developments followed quickly (primarily in England and the United States) triggered by military needs during the war.

After World War II the groundwork was prepared so that quantum molecular science could make heavy use of digital computers and computational chemistry could develop. International summer schools in Quantum Chemistry flourished in the late 1950s and 1960s. The use of the new “high-tech” instrument to finally solve (with well defined approximations) the mathematical equations Dirac had referred to, and to obtain in this way actual molecular data which were until then only obtainable from experiments, became a very attractive field for young people. So in the first decades after the war the primary users of computers for purposes of basic science were quantum chemists.

Several reviews on the development of computational chemistry in various countries, which shine light on these times, are available in the literature (2) as well as a booklet on the early time in Sweden (3).

- (1) P A M Dirac, *Proc. R. Soc. London, Ser. A*, **123**, 714 (1929), Quantum Mechanics of Many-Electron systems
- (2) J D Bolcer and R B Hermann, in *Reviews in Computational Chemistry*, K B Lipkowitz and D B Boyd, eds, VCH Publishers, New York, 1994. Vol.5, pp.1-63 (USA), Vol.10, pp.271-316 (UK), Vol 12, pp 367-380 (France), Vol.15, pp.213-299 (Canada), Vol.18, pp.257-291 (Germany)
- (3) A Fröman and J Linderberg, 2007, Uppsala University Library, Box 510, SE-75120 Uppsala, Sweden. Inception of Quantum Chemistry at Uppsala



City of Menton



2.2 The Beginning of the Academy

In France the first scientific meeting in quantum chemistry after the war, the “Colloque de Chimie Quantique” was held 1948 in Paris to give French chemists the opportunity to interact with world leaders (R.S. Mulliken, C.A. Coulson, H.C. Longuet-Higgins and others) of the new science. The first summer school in France was organized under the auspices of NATO in 1963 by R. Daudel in Menton, in exceptionally nice and inspiring surroundings. Scientists and students were obviously very welcome to the city of Menton with its mayor Francis Palméro and had very fruitful weeks of studies. This was considered an excellent opportunity to arrange further summer schools in Menton, organized by A. and B. Pullman and R. Daudel in years to follow (1965, 1970).

The year 1967 seemed to be the perfect time for a new step to make the Quantum Molecular Science better visible in the concert of the other branches of chemistry. This was 40 years after Walter Heitler and Fritz London (working with Erwin Schrödinger in Zürich) had published their article in *Zeitschrift für Physik* “Wechselwirkung neutraler Atome und Homöopolare Bindung nach der Quantenmechanik” (*Z. Physik*, (1927), **44**, 455), work which is regarded by many as the birth of quantum chemistry. The international pioneers Raymond Daudel (France), Per-Olov Löwdin (Sweden), Robert Parr (USA), John A. Pople (UK and USA) and B. Pullman (France), under the inspiration and support of Nobel Laureate Louis de Broglie (France) created the International Academy of Quantum Molecular Science. The mayor Francis Palméro was very instrumental for the decision to have Menton as the site of the new Academy and proposed the Villa Maria Serena in Menton as its headquarters. Palméro was mayor of Menton from 1953 until 1977 and Sénateur des Alpes-Maritimes from 1971 until his death 1985. His support of the Academy and his hospitality was continued by his successors in Menton. The Academy members meet up to the present day every year at the splendid Villa; since 1989 with the support of Mayor Jean-Claude Guibal, who is also “député de la quatrième circonscription des Alpes-Maritimes” since 1997 (reelected 2007).

The villa Maria Serena was built in the 1880 by Charles Garnier, the architect of the Garnier opera in Paris and of the Casino in Monte-Carlo, for his friend Ferdinand de Lesseps, who built both the Suez and the Panama canals. The last owner, Henri König, donated the villa and its beautiful parks in 1947 to the city of Menton with the words “After having spent 17 happy years in Menton, I leave Maria Serena to the city as a token of my gratitude”.



Park of Villa Maria Serena



Memorial stone at the Villa Maria Serena

The purpose of the Academy is stated in its first meeting: to further the development of Quantum Molecular Science by, for example:

- (1) Exchange of information on big computer programs
- (2) Exchange of information on international meetings
- (3) Award of a prize to a brilliant young scientist, who has carried out important research within the field

The first two points seemed to be obvious for the established scientists, given the situation of the field at that time. The third point meant an important incentive for young people to bring original ideas and new techniques into the fast developing field. For the winners of this prize it meant high international recognition and support in their careers.

Since Menton was chosen as headquarters, the statutes of the Academy are formulated in the French and English language. The letter Ψ , representing the quantum mechanical wavefunction, was chosen as Logo for the Academy. The founding fathers originally added the ring on top of Ψ to suggest a delocalized bond. But very soon another interpretation appeared to show the special relation of the Academy to its site in Menton: the ellipse is taken as a symbol for the lemon which is characteristic for the city of Menton.

2.3 The growing Academy

The first five years....

At the first meeting 1967 the five founding fathers elected immediately 11 new members (Chapter 3.7) All of them were pioneers in the field, three already Nobel Laureates at that time, two of them winning the Nobel Prize later on. The growth slowed somewhat down in the years to follow, since the statutes restricted the number of members under the age of 65 to only 25. Nevertheless, after the first five years (1972) the Academy had already 29 members, and the list reads like WHO is WHO in quantum molecular science. The largest number (11) came from the USA, but in addition to the initial four countries (USA, F, UK, S) seven others (Japan, Germany, Israel, Czechoslovakia, Switzerland, Italy and USSR) were now represented in the Academy. Although most of the members were dedicated to theory, the title of the Academy was chosen wide enough to include also some members doing primarily experimental quantum molecular work. The representation of the countries is also somewhat reflected in the home-countries of the first five medallists, three from the USA and one each from Israel and Poland.

The Academy meetings were important for the exchange of information, as put down in the initial session 1967. In general, the members reported on their work in the area of all-electron calculations, quantum theory of reactivity and quantum studies of biological systems – all topics which are still among the main stream problems to date. The activity of the Academy was significantly broadened in its meeting 1971: the decision was made to organize 1973 in Menton a First International Congress of Quantum Chemistry, on the occasion of the 50th anniversary of the first publication in 1923 of the decisive wave mechanics work of Louis de Broglie.

The next 35 years 1972 - 2007

The importance of quantum molecular science became rapidly evident in many fields of chemistry, pharmacy, material science, selected fields of physics and lately also for life sciences. Professorships and chairs were created at many universities and research institutions throughout the world. The field boomed, international exchange of information became routine and international exchange of young people followed. The first generation of quantum chemists became experts and created their own schools of students at various sites in many countries. So it was time to increase the number of Academy members and relax the restriction of only 25 scientists below the age of 65. In 1982 this number was increased from 25 to 30, in 1992 Article 5 of the Statutes was amended so that the number of members below 65 was set to 35.

It was obvious that the number of scientists in the field increased steadily worldwide so that the restriction to 35 members below the age of 65 years could not be retained. A look at other international academies showed that these had similar problems and in most cases had increased their limit for the maximum number of members. In addition, the distinction (introduced 1976) between “ordinary” members (those under the age of 65) and “senior” members (above the age of 65) was considered as discrimination against age. For these reasons it was decided at the Academy meeting 2006 to decide via a postal vote whether Article 5 of the Statutes should be eliminated entirely. It was not expected, however, that the number of members will drastically increase, since the extremely high quality and worldwide recognition remains the basic criterion for election into the Academy. The vote was undertaken and a clear 2/3 majority was for the elimination of Article 5. This means that since 2007 the Academy has formally no longer a restriction for the number of members.

In spring 2007 the Academy had a total of 88 members coming from 20 countries. 33 were below the age of 65 and four reached this age during the year. The number of members from the USA is still the largest (29), and 12 countries of Europe are now represented (Belgium, Denmark, Czech Republic, Finland, France, Germany, Italy, Netherlands, Norway, Poland, Sweden and the United Kingdom) in addition to Canada, Russia and the Asia-Pacific area Australia, China, India and Japan. The scientists in the latter region have become extremely active in recent years and have founded 2004 the Asia-Pacific Association of Theoretical and Computational Chemists (APATCC) which held its first Conference in 2004 in Japan, followed by conferences in Thailand (Bangkok 2005), China (Beijing 2007) while the 4th in this series is planned for 2010 in Singapore. It is certainly expected that the influence of the Asia-Pacific Region on theoretical chemistry will increase considerably in the future and that an appropriate representation of this area will also be seen in the Academy.

One part of the Academy meetings was obviously always devoted to the election of new members and to the selection of the medallist. This part was generally followed by a minisymposium at which members presented results of their work. In addition, it was the responsibility of the Academy meetings to select the sites and the organizers of the International Congresses of Quantum Chemistry and to suggest and agree on possible invited speakers of such Congress. Generally, the medal winner and the newly elected members were invited to give a lecture at the next Congress while Academy members were expected not to deliver main lectures at two consecutive Congresses. In this way young scientists obtained a special opportunity to present results of their work. 1991 was the last meeting at which all five founding members were present.

1991 Academy Meeting at the Villa Maria Serena



Front row: L Radom, R Pauncz, J Linderberg, S Peyerimhoff, A Pullman, R McWeeny, I Fischer-Hjaltners, W Goddard
 Middle rows: A Veillard, J Jortner, P Pulay, J Pople, R Hoffmann, W Kolos, J Koutecky, A Buckingham, B Pullman, I Shavitt, E Davidson, P-O Lowdin, K
 Ruedenberg, K Morokuma, R Marcus, R Lefebvre, J Cizek, G Hall, N Handy
 Back row: M Karplus, R Zahradnik, W Kutzelnigg, R Parr, J Michl, W Miller, R Daudel

In more recent years the emphasis in the presentation of individual members in the form of minisymposia was shifted to more general aspects, e.g. the evaluation of present quantum mechanical methods and their future impact, discussions in which direction the field will go and in which areas of quantum molecular science advances could be expected. Likewise discussion on the feasibility of exchange of innovative teaching programs for students was a topic, a major step compared to the first ambition of 1967 to exchange computer programs. The question will also be pursued whether it is time for this International Academy to play a role in science policy.

The growing Academy has become very international. Nevertheless, its meeting location remains Menton (except in the years of the International Congress). The hospitality of the city of Menton is very much appreciated.



Thanks to Mrs Jausseran for her service at the Villa (2007).

Dinner at the Villa Serena: Welcome by Mrs. Filippi, Representing the Deputy-Mayor of Menton (2007)



2.4 The years 2007 – 2017

Under the presidency of Sigrid Peyerimhoff, there was a revival to strengthen the links between the Academy and the city of Menton in the spirit of one the founding Member, Raymond Daudel and to recognize the efforts made by Menton to host our Academy meeting at considerable expense for the city (free access to the Villa Serena, invitation to the Mayor's banquet). In 2007, talks were given to high-school students on subjects of general interest. This session was opened by a representative of Menton and 35- 50 people attended.

■ conférence —

Mieux comprendre la chimie quantique

L'Académie Internationale des Sciences moléculaires quantiques, en collaboration avec la ville de Menton, propose une conférence de vulgarisation qui aura lieu à la Villa Maria Serena, le vendredi 6 juillet, à 18 heures.

Deux pionniers de la chimie quantique en Belgique, Jean-Claude Lorquet, professeur émérite à l'Université de Liège, et Jean-Marie André, professeur à l'Université de Namur, feront une courte présentation des sujets suivants : « Qu'est-ce qu'une réaction chimique? Comprendre et orienter les affinités électives » et « Matériaux polymères et plastiques. Avantages et risques, du « celluloïd » à l'accident de la navette spatiale Challenger ».

Suivra une séance de questions posées par le public.

Rappelons que l'IAQMS a

été établi en 1967 son siège à Menton, où elle se réunit une fois par an.

Ses membres sont choisis parmi d'imminents scientifiques venus du monde entier.

L'académie offre un centre de rencontre favorisant les contacts et les collaborations au niveau international par une évaluation régulière des principaux développements, des avancées et des directions de recherche prometteuses dans le domaine de la chimie quantique.

Aujourd'hui, les membres de l'académie proviennent de vingt pays différents, et six de ses membres sont français.

Savoir +

■ Entrée libre.

Renseignements : service des affaires culturelles au 04.92.10.50.83.

Jean-Marie André and Jean-Claude Lorquet were active in establishing close contacts with the Lycée Pierre et Marie Curie at Menton. Conferences with the Lycée Pierre et Marie Curie were organized on a regular basis until 2011. Besides Jean-Marie André and Jean-Claude Lorquet, already cited, Josef Michl, Michel Dupuis and Pekka Pyykkö delivered highly appreciated lectures. In 2012, a new Menton committee has been formed and includes J.-M. André, J.-C. Lorquet, Andreas Savin, and Odile Eisenstein, who will serve as the coordinator. It quickly appears that this committee would have interaction with the ICQC 2018 Menton organizing committee.

In the same way to improve the links with the city of Menton, an Honorary Medal was awarded by President Peyerimhoff in 2008 to Jean-Claude Guibal, Mayor of Menton since 1989. The citation is “*Jean-Claude Guibal, Maire de Menton, en reconnaissance des services rendues à*

l'IAQMS, 2008". This was an occasion of a very nice official reception for all the Members of the Academy at the City Hall in the impressive "salle du conseil".

■ sciences

Jean-Claude Guibal honoré par l'Académie de physique quantique

Les chercheurs de l'Académie internationale des sciences moléculaires quantiques ont décerné, en clôture de la réunion annuelle, une médaille d'honneur à Jean-Claude Guibal, député-maire de Menton. A cette occasion, Sigrid Peyerimhoff, la présidente du centre de recherches fondé à Menton et établi à la villa Maria Serena (promenade Reine- Astrid), a gratifié le maire de sa contribution. La cérémonie s'est déroulée dans la salle du conseil de l'hôtel de ville, en présence d'une trentaine de convives.

« Touché, ému » par la distinction, le député-maire s'est déclaré très favorable à la poursuite de cette collaboration. Jean-Claude Guibal a rappelé combien la présence de ce savoir intellectuel « stimule et irrigue » la ville. Le premier magistrat a par ailleurs invité les chercheurs à sortir de leur humble réserve, à être « plus exigeant » avec une municipalité « pas tout à fait à la hauteur de ce que vous représentez ».

Créée en 1967 sous l'égide du duc Louis de Broglie, l'Académie, composée de plus de 90 membres (dont six Français), est un centre international de recherches et de rencontres. Elle évalue et met en perspective les avancées de la science moléculaire quantique, domaine en expansion qui se penche sur l'étude de matériaux nouveaux, telles les propriétés électroniques.

Le député-maire de Menton a reçu samedi 5 juillet une médaille d'honneur, hommage décerné par Sigrid Peyerimhoff, présidente de l'Académie des sciences moléculaires quantiques de Menton. (Photo Olivier Poisson)

savoir +
Site Internet www.iaqms.org

Considering the mission of the Academe, *i.e.* article 1 of the Statutes “*encourage the development of the applications of wave mechanics to the study of molecular phenomena*” a survey was initiated by the Academy 2008 to investigate how the development of Quantum Molecular Science (QMS) has proceeded in the various countries throughout the world. The goal was to give an overview of the present status of QMS in various countries, to spot the most important trends in the field and to assess the influence of QMS on neighbouring areas. In addition the financial funding of research in various countries, the situation in the education and the possibilities of young researchers on the job market were considered.

Members of the Academy in various countries summarized their knowledge and experience. In countries not represented in the Academy some research groups were addressed to contribute their opinion based on a questionnaire. Response came from Oceania (Australia and New Zealand), Asia (Israel, Japan, Korea, PR China, Thailand, Taiwan) North America (USA, Canada, Cuba), South America (Argentina, Chile, Columbia), Northern Europe (Denmark, Finland, Norway, Sweden, Estonia, Ukraine, Russia), Central and western Europe (Czech Republic, Slovakia, Poland, Hungary, Slovenia, Austria, UK, The Netherlands, Belgium, France, Germany, Switzerland), Southern Europe (Italy, Spain and Greece), Africa (Morocco, Tunisia, Algeria, South Africa).

Since the foundation of the Academy the field has broadened enormously, due to advances in theory and in the computational resources. Today many of the applications of QMS are used parallel to experimental research. With the study of large molecules QMS has spread into many fields like material science, biochemistry, drug design, catalysis and surface science.

The mixing of quantum mechanics QM (original term wave mechanics) with classical (molecular mechanics) methods and statistical mechanics lead to QM/MM methods, Monte Carlo (MC) and Molecular Dynamics (MD) simulations. So the original term of the founding members has evolved into the terms “quantum Chemistry”, Theoretical Chemistry”, Computational Chemistry”.



Applications with existing programs are numerous and are undertaken in all countries surveyed. Major topics are the study of synthesis and stability of new materials, catalysis, the reaction of enzymes, drug design, energy storage, control of chemical reactions, atmospheric and environmental chemistry, spectroscopic parameters and properties of interstellar media. Method development is more restricted to a smaller number of research groups. The financial support is very heterogeneous in the various countries. A definite need for a competent education in computational chemistry for students in all branches of chemistry was recommended to prevent “incompetent number producing”.

Details of the “Survey 2009, Quantum Molecular Science in the World” together with two appendices listing sites, prominent scientists and their research interests are on the Academy’s home page. (“Relations”). The data have not been updated since 2011.

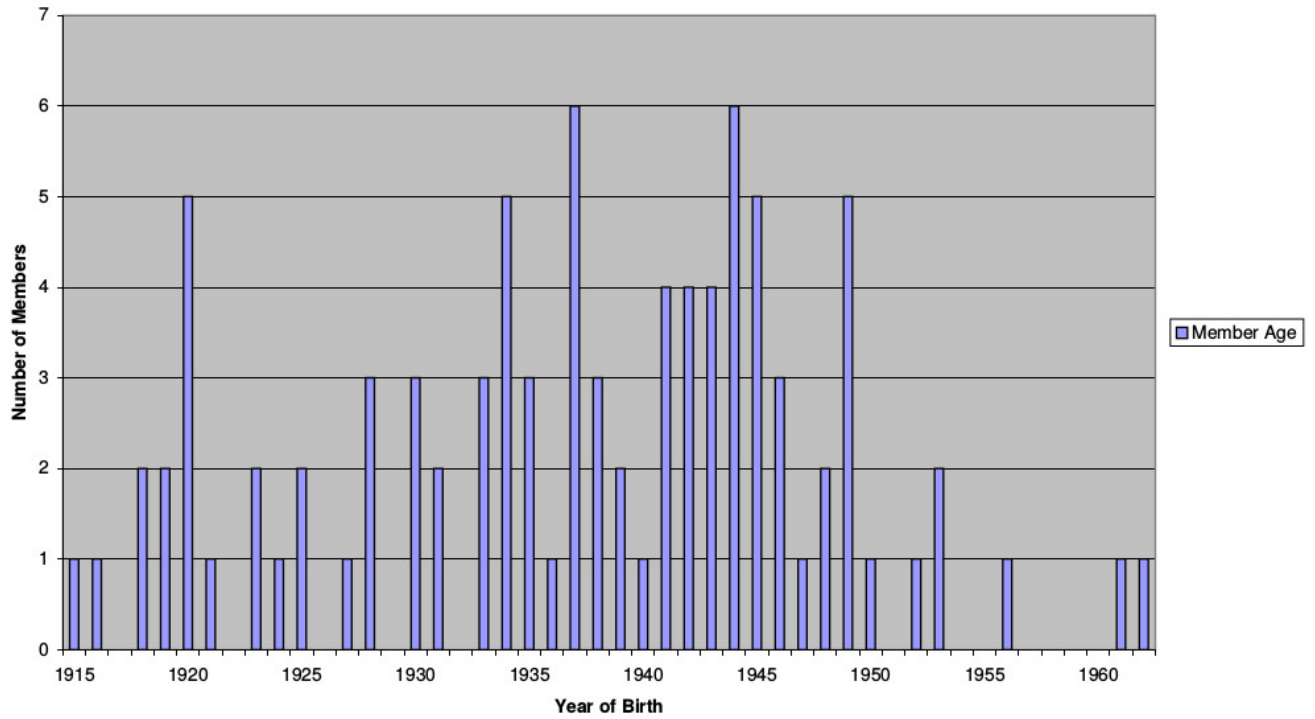
The Academy meeting in the summer of 2007 was the first one at which the number of new members to be elected was not restricted any more by Article 5 of the Statutes. The increase in the number of members in the years to follow can be seen from the two histograms which give the distribution of members according to age. The Academy has grown from 91 members in January 2008 to 121 members in January 2017. It is obvious that most members are now above (or at) the age of 65, but a noticeable number of members born later than 1960 have been appointed within the past 10 years.

Distribution of members in countries

country	Year 2008			Year 2017
	Age above 65	Below 65	total	total
USA	23	10	33	48
Canada	1	2	3	4
Australia	1	1	2	2
New Zealand				1
China	1		1	2
India		1	1	1
Japan	2	3	5	6
Korea				1
Russia	2		2	2
Israel	3	1	4	5
Austria				1
Belgium	1	1	2	2
Czech Republic	2		2	2
Denmark	1	1	2	3
Finland	1		1	1
France	4	1	5	6
Germany	5	5	10	12
Italy	3		3	4
Netherlands	2	2	4	4
Norway		1	1	2
Poland		1	1	1
Slovakia				2
Sweden	2	1	3	1
Switzerland				1
UK	4	2	6	7
Sum	58	33	91	121

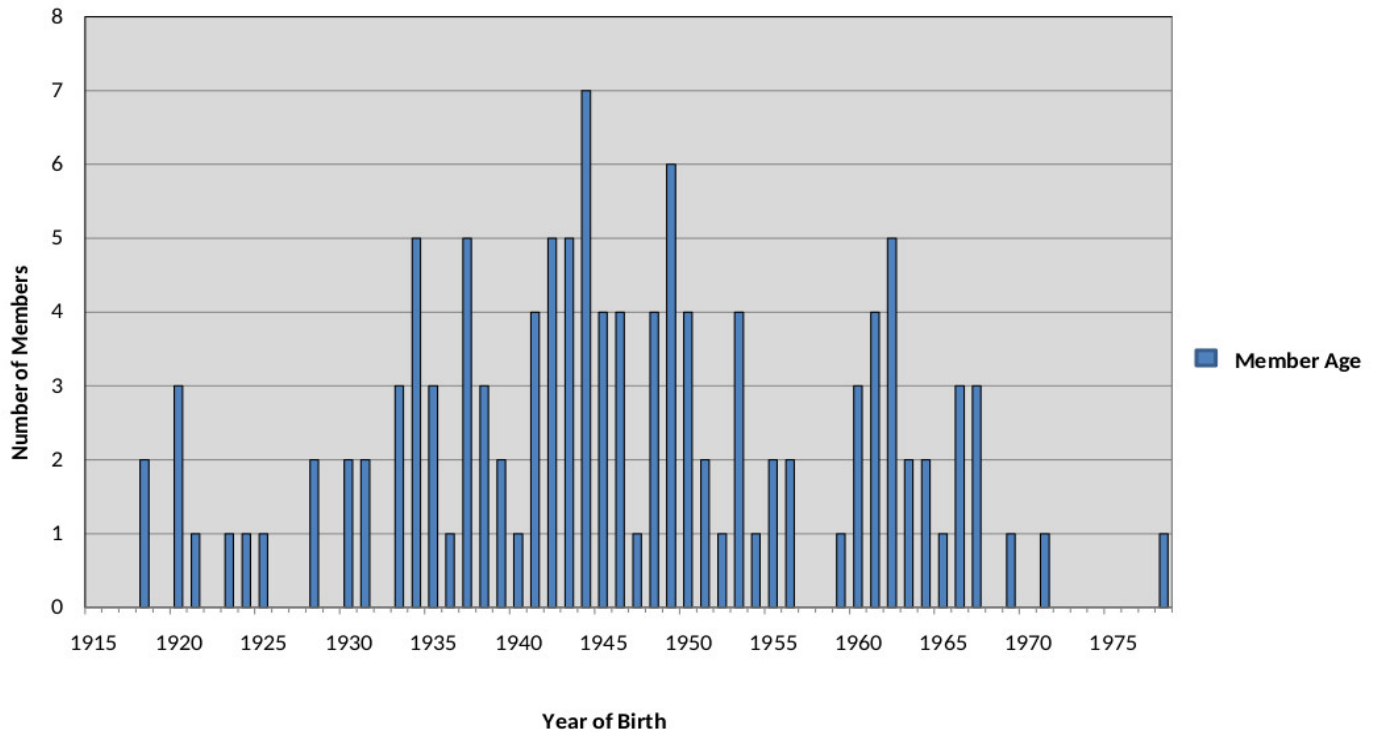
2008

Member Age



2017

Member Age (Total of 121)



The distribution of members with respect to countries is presented in the Table. The largest number of members of our Academy work in the USA. Within the past 10 years scientists of New Zealand, Korea, Austria, Slovakia and Switzerland, *i.e.* countries previously not represented in the Academy, were elected.

The election procedure for members and the medalists was thoroughly discussed in several meetings. A Canvassing Committee was established 2013 to identify and secure nominations from underrepresented groups including age, gender, geography and subdisciplines, headed by Gustavo Scuseria. Its efforts lead to a larger variety of nominations. The first consequence was the election of 6 women in the years from 2014 to 2016. At present the Academy lists 10 women among 121 members. Since 2016 the Canvassing Committee is elected by secret ballot at the annual Academy Meeting and will serve for one year.

As in previous years the preparation of the International Congresses of Quantum Chemistry is an important topic on the agenda of the Academy meetings. The sites, the organizers, the scientific committee are chosen and the invitation of the main speakers is discussed. The medal winners are always invited to speak at the consecutive Congress.

Finally, one special characteristics of the Academy compared to others should also be pointed out. While National Academies are generally financially supported by their state, this International Academy has no regular financial income – not from any state nor from any of the science organisations. There are occasional donations from within the Academy. On such basis it has become possible from 2005 to 2011 to provide a cash price with the Award of the Annual Medal.

2.5 The International Congresses of Quantum Chemistry

The expansion of the field of quantum molecular science may easily be seen from the topics treated at the International Congresses of Quantum Chemistry and their Satellite Meetings (Chapter 3.8), held every 3 years in another part of the world. The site of the Congresses were so far Menton, (I, 1973), New Orleans, USA (II, 1976), Kyoto, Japan (III, 1979), Uppsala, Sweden (IV, 1982), Montréal, Canada (V, 1985), Jerusalem, Israel (VI, 1988), Menton (VII, 1991), Prague, Czech Republic (VIII, 1994), Atlanta, USA (IX, 1997), Menton (X, 2000), Bonn, Germany (XI, 2003), Kyoto, Japan (XII, 2006), Helsinki, Finland (XIII, 2009), Boulder, USA (XIV, 2012) and Beijing, China (XV, 2015). The Congress 2018 will be held in Menton, France.

Already at the very first Congress there was a great interest to attend such an event which represented a new and interesting field to many of the participants. About 400 scientists and students were present at the first Congress 1973 in Menton, coming from almost 40 countries. More triennial international Congresses in this field followed later on, organized by scientific societies, for example by the World Association of Theoretical and Computational Chemists (WATOC, first Congress 1987 in Budapest) and by the International Society for Theoretical Chemical Physics (ISTCP, first Congress 1993 in Girona). Many regional meetings and summer schools (USA, Canada, Asia-Pacific, Germany, Sweden, UK) were introduced over the years. Nevertheless the Congresses supported by this Academy continue to attract researchers of all parts of the world. It is an ideal media to learn about the actual status of the field, method developments and applications, to stimulate contacts, collaborations and friendships between quantum chemists at the world-wide level.

For a long time the number of scientists attending such a Congress was around 500, coming from about 50 nations. In addition many students in the area took the opportunity to attend these lectures and to meet with international speakers. Within the past 10 years the number of participants has increased up to about 1000 (Beijing 2015). The representation of countries, in particular of Eastern Europe and from the former Sowjetunion, was highest at the Congresses in Helsinki and Germany.

The invited lectures of the first four Congresses were published in separate books. Starting 1985 the main lectures, and in some cases also some of the short presentations, appeared in the International Journal of Quantum Chemistry. Since the number of contributions and posters increased considerably over the years (to about 600), the reviewing procedure to guarantee the publication of all contributions within a short period of time became too elaborate; hence the distribution of the Book of Abstracts was eventually considered to be sufficient.

Although the Academy members were elected in the last two decades on the basis of their achievements in theory, the important relation to experiment is always present by inviting a few highly regarded experimentalists to deliver plenary lectures at the Congresses. The pictures show Ahmed Zewail amidst the audience at the XI ICQC in 2003 and the two nobel prize winners A. Zewail and J. A. Pople with the rector K. Borchard of the University of Bonn.



The initial themes formulated at the first Congress, *i.e.* Methods in Quantum Chemistry, Structure and Conformation, Chemical Reactivity, Spectroscopy and Effects of Environment are still in the main stream of research and appear as topics of recent Congresses. The variety of concepts and the accuracy of methods have changed dramatically, however. The molecular systems which can be treated realistically now have hundreds or even thousands of atoms and chemical accuracy (in the order of a kcal/mole or less) can be achieved routinely. Time-dependent formulations and Molecular Dynamics play a major role in the theory of chemical



reactions and in the interaction of light with matter. The study of environmental effects requires still considerable work. The area of applications has become large, and glancing through Chapter 3.8 will give an impression of the wide variety of possibilities in today's application of Quantum Molecular Science. Research in many areas of chemistry, biophysics, atmospheric physics and

chemistry, material and condensed phase science nowadays are inconceivable without using quantum theory.

2.6 Thoughts in Retrospect

The Academy was founded to provide a forum for worldwide contact and collaboration and a periodical evaluation of the many developments, advances and promising directions of research in the broad field of Quantum Molecular Science.

In the past 50 years the field has grown tremendously. Progress in many fields of chemistry, parts of physics and even life sciences are no longer conceivable without quantum chemical calculations and analysis. The International Congresses, arranged by the Academy, provide over the years an excellent opportunity to discuss on an international level the most recent developments and results in the field. The Award of the Medal to support the pioneering work of a young person below the age of 40 is always a big encouragement and also sets a sign which scientific development seems to be going in a promising direction.

The five founding fathers did not decide to start national academies, which might have been the more obvious thought of people at that time. They saw the future in world-wide cooperation. The first 50 years of the Academy have been extremely successful. We hope the Academy can in coming decades live up to the standards set up so far.



Academy meeting 2007: Last rows (left to right) J Michl, J Tomasi, J Cizek, E J Baerends, A v d Avoird, K Hirao, B Roos, H J Werner, P skyCársky, M Gordon, M Dupuis
 Middle rows: P Pyykkö, B Jeziorski, W Yang, W Kutzehnigg, W Lester, R Lefebvre, W Meyer, S Kato, J C Lorquet
 First 2 rows: N C Handy, D Mukherjee, R Pannuz, C C J Roothaan, R Levine, S D Peyerimhoff, M Robb, J M André, T Helgaker, E Clementi, R Barlett



Academy meeting 2016: 1st P. Schwerdtfeger, P. Pykkö, J. Michl, S. Peyertshoff, 2nd T. Helgaker, L. Radom, K. Ruedenberg, S. Ten-No, 3rd K. Szalewicz, U. Röhlisberger, L. Bartlett, P. Gill, S. Shaik, W. Meyer, 4th M. Gordon, W. Liu, J.-C. Lorquet, M. Dupuis, P. Čárský, 5th A. Krylov, B. Jezioriski, P. Pulay, H. Nakatsuji, S. Hirata, M. Urban, 6th W. Nieuwpoort, B. Mennucci, R. Broer, H.-J. Werner, 7th H.F. Schaefer, H.-J. Werner, O. Eisenstein, G. Scuseria, S. Grimme

3 DOCUMENTS

All documents until 2007 collected by Nicholas C. Handy

3.1 Members of the Academy

(January 1, 2017)

	<u>Country of Residence at time of election</u>	<u>Date of Birth</u>	<u>Date of Election</u>
A			
ALAVI, Alii	UK, Germany	1966	2016
ALEXANDER, Millard H	USA	1943	2017
ANDRÉ, Jean-Marie	Belgium	1944	2002
B			
BAERENDS, Evert-Jan	Netherlands	1945	1999
BARONE, Vincenzo	Italy	1952	2008
BARTLETT, Rodney J	USA	1944	1991
BASILEVSKY, Mikhail V	Russia	1935	1991
BECKE, Axel D	Canada	1953	2000
BOWMAN, Joel M.	USA	1948	2013
BREDAS, Jean-Luc	USA	1954	2011
BROER-BRAAM, Ria	Netherlands	1951	2014
BUCKINGHAM, A David	UK	1930	1985
C			
CARSKY, Petr	Czech Republic	1942	1994
CARTER, Emily A	USA	1960	2009
CEDERBAUM, Lorenz S	Germany	1946	1998
CEPERLEY, David M	USA	1949	2013
CHAN, Gamet Kin-Lic	USA	1978	2014
CIZEK, Jiri	Canada	1938	1987
CLARY, David C	UK	1953	1998
CLEMENTI, Enrico	Italy	1931	1994
D			
DAVIDSON, Ernest R	USA	1936	1981
DOMCKE, Wolfgang	Germany	1948	2003
DUNNING, Thom	USA	1943	2015
DUPUIS, Michel	USA	1949	2005
E			
EISENSTEIN, Odile	France	1949	2006
F			
G			
GAO, Jiali	USA	1962	2016
GAUSS, Jürgen	Germany	1960	2009
GILL, Peter	Australia	1962	2015
GODDARD, William A	USA	1937	1986
GORDON, Mark S	USA	1942	2004
GRIMME, Stefan	Germany	1963	2013
H			
HALL, George G	UK	1925	1974
HAMMES-SCHIFFER, Sharon	USA	1966	2014
HEAD-GORDON, Martin	USA	1962	2006
HELGAKER, Trygve	Norway	1953	2005

HELLER, Eric J	USA	1946	1994
HIRAO, Kimihiko	Japan	1945	2002
HIRATA, So	USA	1971	2014
HOFFMANN, Roald <i>(Nobel Prize Winner)</i>	USA	1937	1978
HOUK, Kendall N	USA	1943	2003
J			
JEZIORSKI, Bogumil	Poland	1947	1999
JØRGENSEN, Poul	Denmark	1944	2012
JORGENSEN, William L	USA	1949	2010
JORTNER, Joshua	Israel	1933	1982
K			
KARPLUS, Martin <i>(Nobel Prize Winner)</i>	USA	1930	1967
KIM, Kwang S	Korea	1950	2009
KLOPPER, Wim	Germany	1961	2011
KOSLOFF, Ronnie	Israel	1948	2000
KRESSE, Georg	Austria	1967	2012
KRYLOV, Anna	USA	1967	2015
KUTZELNIGG, Werner	Germany	1933	1990
L			
LEFEBVRE, Roland	France	1928	1990
LESTER, William A	USA	1937	2006
LEVINE, Raphael D	Israel	1938	1987
LEVY, Mel	USA	1941	2009
LIGHT, John C	USA	1934	1994
LINDERBERG, Jan E	Denmark	1934	1982
LIU, Wenjian	China	1966	2014
LORQUET, Jean-Claude	Belgium	1935	1993
M			
MAKRI, Nancy	USA	1962	2010
MALRIEU, Jean-Paul	France	1939	2000
MANOLOPOULOS, David E	UK	1961	2013
MARCUS, Rudolph A <i>(Nobel Prize Winner)</i>	USA	1923	1987
McWEENY, Roy	UK	1924	1973
MENNUCCI, Benedetta	Italy	1969	2014
MEYER, Wilfried E	Germany	1938	1995
MICHL, Josef	USA	1939	1988
MILLER, William H	USA	1941	1985
MOROKUMA, Keiji	Japan	1934	1985
MUKHERJEE, Debashis	India	1946	1997
N			
NAGAKURA, Saburo	Japan	1920	1979
NAGASE, Shigeru	Japan	1946	2008
NAKATSUJI, Hiroshi	Japan	1943	1993
NEESE, Frank	Germany	1967	2012
NIEUWPOORT, Willem C	Netherlands	1931	1996
NIKITIN, Evgueni E	USSR	1933	1987
NOGA, Jozef	Slovakia	1955	2014
NOOIJEN, Marcel	Canada	1963	2016
O			
OLSEN, Jeppe	Denmark	1956	2002
P			
PALDUS, Josef	Canada	1935	1984
PARR, Robert G <i>(Founder Member)</i>	USA	1921	1967
PARRINELLO, Michele	Germany	1945	1995
PAUNCZ, Ruben	Israel	1920	1968

PERDEW, John P	USA	1943	2003
PEYERIMHOFF, Sigrid D	Germany	1937	1986
PULAY, Peter	USA	1941	1990
PYYKKO, Pekka	Finland	1941	1992
R			
RADOM, Leo	Australia	1944	1989
RAGHAVACHARI, Krishnan	USA	1953	2010
RATNER, Mark A	USA	1942	2003
RICE, Julia	USA	1960	2016
ROBB, Michael A	UK	1944	2000
ROOTHAAN, Clemens C J	USA	1918	1967
RÖTHLISBERGER, Ursula	Switzerland	1964	2015
RUEDENBERG, Klaus	USA	1920	1973
S			
SALEM, Lionel	France	1937	1982
SAUE, Trond	Norway	1964	2016
SAVIN, Andreas	France	1950	2012
SCHAEFER, Henry F	USA	1944	1984
SCHATZ, George C	USA	1949	2001
SCHLEGEL, H Bernhard	USA	1951	2011
SCHWERDTFEGER, Peter	New Zealand	1955	2012
SCUSERIA, Gustavo E	USA	1956	2009
SHAIK, Sason	Israel	1948	2015
SHUAI, Zhigang	China	1962	2008
SIEGBAHN, Per E M	Sweden	1945	1994
STANTON, John F	USA	1961	2009
SZALEWICZ, Krzysztof	USA	1950	2010
T			
TEN-NO, Seiichiro	Japan	1965	2012
THIEL, Walter	Germany	1949	2007
TOMASI, Jacopo	Italy	1934	1999
TRUHLAR, Donald	USA	1944	2006
TULLY, John	USA	1942	2000
U			
URBAN, Miroslav	Slovakia	1942	2008
V			
Van der AVOIRD, Ad	Netherlands	1943	1997
VEILLARD, Alain	France	1934	1987
VOTH, Gregory	USA	1959	2013
W			
WARSHEL, Arieh <i>(Nobel Prize Winner)</i>	USA	1940	2015
WERNER, Hans-Joachim	Germany	1950	2001
Y			
YANG, Weitao	USA	1961	2006
Z			
ZAHRADNIK, Rudolf	Czechoslovakia	1928	1982

3.2 Members of the Academy deceased (January 1, 2017)

	<u>Country of Residence at time of election</u>	<u>Date of Birth</u>	<u>Date of Election</u>	<u>Deceased</u>
A				
AHLRICH, Reinhart	Germany	1940	1993	2016
B				
BATES, David R	UK	1916	1985	1994
De BROGLIE, Louis (<i>Nobel Prize Winner</i>)	France	1892	1967	1987
BOYS, S Francis	UK	1911	1969	1972
C				
COULSON, Charles A	UK	1910	1967	1974
CRAIG, David P	Australia	1919	1977	2015
D				
DALGARNO, Alexander	USA	1928	1993	2015
DAUDEL, Raymond (<i>Founder Member</i>)	France	1920	1967	2006
DAVYDOV, Alexander S	USSR	1912	1975	1993
DEWAR, Michael J S	USA	1918	1989	1997
E				
EYRING, Henry	USA	1901	1969	1981
F				
FISCHER-HJALMARS, Inga	Sweden	1918	1983	2008
FOCK, Vladimir A	USSR	1898	1972	1974
FUKUI, Kenichi (<i>Nobel Prize Winner</i>)	Japan	1918	1970	1998
G				
GÁSPÁR, Rezső	Hungary	1921	1974	2001
H				
HANDY, Nicholas C	UK	1941	1988	2012
HARTMANN, Hermann	Germany	1914	1975	1984
HEITLER, Walter H	Switzerland	1904	1970	1981
HEILBRONNER, Edgar	Switzerland	1921	1976	2006
HERZBERG, Gerhard (<i>Nobel Prize Winner</i>)	Canada	1904	1973	1999
HIRSCHFELDER, Joseph O	USA	1911	1968	1990
HUCKEL, Erich	Germany	1896	1968	1980
HUND, Friedrich	Germany	1896	1969	1997
J				
K				
KASHA, Michael	USA	1920	1992	2013
KATO, Shigekil	Japan	1949	2004	2010

KOHN, Walter <i>(Nobel Prize Winner)</i>	USA	1923	1991	2016
KOLOS, Włodzimierz	Poland	1928	1988	1996
KOTANI, Masao	Japan	1906	1967	1993
KOUTECKY, Jaroslav	Czechoslovakia	1922	1969	2005
L				
LONGUET-HIGGINS, H. Christopher	UK	1923	1967	2004
LOWDIN, Per-Olov <i>(Founder Member)</i>	Sweden	1916	1967	2000
M				
MATSEN, Frederick A	USA	1913	1987	2006
McCONNEL, Harden M	USA	1927	1967	2014
MULLIKEN, Robert S <i>(Nobel Prize Winner)</i>	USA	1896	1967	1986
N				
O				
P				
PAULING, Linus <i>(Nobel Prize Winner)</i>	USA	1901	1967	1994
POPLE, John A <i>(Nobel Prize Winner & Founder Member)</i>	USA	1925	1967	2004
PULLMAN, Alberte	France	1920	1967	2011
PULLMAN, Bernard <i>(Founder Member)</i>	France	1919	1967	1996
R				
ROOS, Björn-Olof	Sweden	1937	1991	2010
S				
SANDORFY, Camille	Canada	1920	1974	2006
SCHLEYER, Paul v R	Germany	1930	1992	2014
SCROCCO, Eolo	Italy	1916	1971	2012
SHAVITT, Isaiah	USA	1925	1985	2012
SIMONETTA, Massimo	Italy	1920	1976	1986
SLATER, John C	USA	1900	1967	1976
T				
TANG, Au-chin	China	1915	1981	2008
TELLER, Edward	USA	1908	1979	2003
V				
Van VLECK, John H <i>(Nobel Prize Winner)</i>	USA	1899	1968	1980
W				
WILSON, E. Bright	USA	1908	1968	1992
Y				
Z				
ZIEGLER, Tom	Canada	1945	2007	2015

3. 3 Statutes of the Academy (English)

(Revised July 6, 2002)

Article one

In order to encourage the development of the applications of wave mechanics to the study of molecular phenomena, an International Academy of Quantum Molecular Sciences is founded.

Article two

The existence of the Academy is unlimited. The headquarters are in MENTON, France.

Article three

The purposes of the Academy are entirely scientific and exclude all social, political or commercial activities.

Article four

The Academy is composed of persons chosen amongst the scientists of all countries who have distinguished themselves by the value of their scientific work, their role of pioneer or leader of a school and have most contributed to the advancement of quantum molecular sciences.

Article five Deleted 2007

The number of members under the age of sixty-five on the last day of December of the year the decision is made cannot exceed **thirty-five**.

Article six

The Governing Body of the Academy includes the President, the Vice-President and three other members. The members of this body are chosen amongst the members of the Academy during a meeting of the Academy. The elections are held by secret ballot. For the first two rounds the absolute majority is necessary for election, for the third round a relative majority is sufficient. The term of office for members of the Governing Body is three years.

Article seven

New members of the Academy are chosen by the existing members. Each election involves the following steps:

1. Prior to the Academy meeting the President prepares a list of candidates for election based on the written proposals of the members of the Academy, accompanied by supporting documents.
2. At each election session the Governing Body decides the maximum number of new members which may be elected at that session.
3. A vote is held for the **nomination** for election. In order to be nominated, a proposed candidate must receive an **absolute majority** of the votes of members of the Academy present at the meeting. The voters inscribe **at most as many names** on the voting list as there are available places. New rounds of voting are held until the number to be elected is nominated or no majority is achieved for any further nominee after **three consecutive votes**.
4. A final vote is held for the **election**. The required majority is **two thirds** of votes of the members present at the meeting. If the number of the nominees is smaller or equal to the number of available places, the vote is unique, each member being able to vote for as many of the nominated candidates as he wishes. If the number of the nominees is greater than the number of available places, the voters inscribe at most as many names on the voting list as there are available places. The vote stops when all the available places are filled up or when no two third majority is obtained on any name after **three consecutive votes**.

Article eight

The Academy meets at least once a year. Elections to the Governing Body and of new members can only take place during a meeting of the assembly of the Academy.

Article nine

In the course of this assembly the Academy may decide to award a prize to an eminent scientist in the field of Quantum Molecular Science. The choice is preferably made on the following criteria:

- 1) The candidate should be 40 years old or less on the first day of January of the year the decision is made;
- 2) The candidate should be the author of one or more highly original papers which have an evident importance for Quantum Molecular Science.

The recipient is chosen by the same procedure as that followed for the election of new members. The prize winner can use the title of Laureate of the International Academy of Quantum Molecular Science.

Article ten

The members of the Academy can on important occasions wear the insignia of the Academy. This insignia is made up of the letter psi attached to a ring which suggests a delocalized bond and is worn as a tie with a ribbon made after the colors of the city of MENTON.

Article eleven

These statutes can only be modified by a vote of **two-thirds** of the votes of the members who vote. Vote by mail is permitted.

3.4 Statuts de l'Académie (French)

(Révisé le 6 juillet 2002)

Article Premier

Afin de favoriser et d'encourager le développement des applications de la Mécanique Ondulatoire à l'étude des phénomènes moléculaires, une Académie Internationale des Sciences Moléculaires Quantiques est fondée.

Article Second

Sa durée est illimitée. Son siège est à MENTON (France).

Article Troisième

Ses préoccupations sont entièrement scientifiques et excluent toute activité sociale ou politique ou commerciale.

Article Quatrième

L'Académie est constituée par un ensemble de personnalités choisies parmi les chercheurs scientifiques de tous les pays du monde qui par leur découvertes, leur rôle de pionnier, et de chef d'école, ont le plus contribué au développement des sciences moléculaires quantiques.

Article Cinquième Effacé 2007

Le nombre des Membres d'âge supérieur à 65 ans à la date du 31 décembre de l'année où la décision est prise ne peut dépasser **TRENTE-CINQ**.

Article Sixième

Le Bureau de l'Académie comprend un Président, un Vice-Président et trois autres membres. Les membres de ce Bureau sont choisis parmi les Académiciens au cours d'une assemblée de l'Académie.

Les votes se font au bulletin secret. L'élection au cours des deux premiers votes est acquise à la majorité absolue des voix. Au troisième tour de scrutin la majorité relative suffit. Le mandat du Président et du Vice-Président est de trois ans. Le mandat des autres membres du Bureau est également de trois ans.

Article Septième

Les nouveaux Membres de l'Académie sont choisis par les Membres existants. Chaque élection procède selon les étapes suivantes :

- 1) Avant la réunion de l'Académie, le Président établit une liste de candidats à l'élection basée sur les propositions écrites des Membres de l'Académie accompagnées des documents justificatifs.
- 2) A chaque session d'élections, le Bureau décide du nombre maximum de nouveaux Membres pouvant être élus à cette session.
- 3) Un premier tour de scrutin a lieu, portant sur la **NOMINATION** en vue de l'élection. Afin d'être «**Nominé**», un candidat proposé doit obtenir la **MAJORITE ABSOLUE** des votes des Membres de l'Académie présents à la réunion. Les votants inscrivent sur leur Bulletin autant de noms **AU PLUS** qu'il y a de places à pourvoir. De nouveaux tours de scrutin ont lieu jusqu'à ce que le nombre maximum de candidats à élire soient **Nominés** OU que aucun candidat n'ait atteint la majorité après **TROIS TOURS** consécutifs.
- 4) Un vote final a lieu pour l'**ÉLECTION**. La majorité requise est ici des **DEUX TIERS** des membres présents. Si le nombre de **Nominés** est **INFÉRIEUR** ou **ÉGAL** au nombre de places disponibles, le vote est unique, chaque votant pouvant voter pour autant de **Nominés** qu'il le désire. Si le nombre de **Nominés** est **SUPÉRIEUR** au nombre de places disponibles, les votants inscrivent sur leur bulletin autant de noms de **Nominés** qu'il y a de places disponibles. Le vote cesse quand tous les sièges disponibles sont pourvus ou quand la majorité des deux-tiers n'est atteinte sur aucun nom après **TROIS TOURS** de scrutin consécutifs.

Article Huitième

Les Académiciens se réunissent au moins une fois par an. Les élections du Bureau, des nouveaux membres, ne sont effectuées qu'au cours d'une assemblée solennelle.

Article Neuvième

Au cours d'une assemblée, l'Académie peut décider d'attribuer un **PRIX** à un Scientifique éminent dans le domaine des Sciences Moléculaires Quantiques. Le choix est fait de préférence selon les critères suivants :

- 1) Le candidat ne doit pas avoir 40 ans révolus au premier janvier de l'année où la décision est prise.
- 2) Le candidat doit être l'auteur d'un ou plusieurs mémoires très originaux ayant une importance évidente pour les Sciences Moléculaires Quantiques. Le lauréat est choisi en suivant la même procédure que dans l'élection des Membres. Le lauréat peut utiliser le titre de Lauréat de l'Académie des Sciences Moléculaires Quantiques.

Article Dixième

Au cours d'occasions solennelles, les Membres de l'Académie Internationale des Sciences Moléculaires Quantiques peuvent porter un insigne. Cet insigne est constitué par la lettre psi attachée à un anneau évoquant une liaison délocalisée et portée en cravate à l'aide d'un ruban aux couleurs de la ville de MENTON.

Article Onzième

Ces statuts ne peuvent être modifiés que par un vote des **DEUX-TIERS** des Membres votants. Le vote par correspondance est autorisé.

3.5 Members of the Bureau

(1967 – 2017)

1967-1970 1970-1973	President: Vice President: General Secretary: Treasurer: Bureau Member	R. Daudel P. O. Löwdin J. A. Pople B. Pullman R. G. Parr
1973-1976 1976-1979	President: Vice President: General Secretary: Treasurer: Bureau Member	B. Pullman R. G. Parr J. A. Pople R. Pauncz R. Daudel
1979-1982 1982-1985	President: Vice President: General Secretary: Treasurer: Bureau Member	P. O. Löwdin A. Pullman M. Simonetta J. Koutecky R. G. Parr
1985-1988 1988-1991	President: Vice President: General Secretary: Treasurer: Bureau Member	A. Pullman J. A. Pople J. E. Linderberg E.R. Davidson R. Hoffmann
1991-1994 1994-1997	President: Vice President: General Secretary: Treasurer: Bureau Member	R. G. Parr K. Morokuma N. C. Handy E.R. Davidson B. Pullman
1997-2000	President: Vice President: General Secretary: Treasurer: Bureau Member	J. A. Pople S. Peyerimhoff N. C. Handy B. O. Roos A. Pullman
2000-2003	President: Vice President: General Secretary: Treasurer: Bureau Member	K. Morokuma S. Peyerimhoff W. H. Miller B. O. Roos A. Pullman
2003-2006	President: Vice President: General Secretary: Treasurer: Bureau Member	K. Morokuma P. Pyykkö W. H. Miller B. O. Roos A. Pullman
2006-2009	President: Vice President: General Secretary: Treasurer: Bureau Member	S. Peyerimhoff P. Pyykkö K. Hirao M. S. Gordon R. J. Bartlett

2009-2012	President: Vice President: General Secretary: Treasurer: Bureau Member	P. Pyykkö J. Michl K. Hirao M. S. Gordon J. M. André
2012-2015	President: Vice President: General Secretary: Treasurer: Bureau Member	J. Michl G. Scuseria H. Nakatsuji M. Dupuis O. Eisenstein
2015-2018	President: Vice President: General Secretary: Treasurer: Bureau Member	J. Michl G. Scuseria H. Nakatsuji M. Dupuis O. Eisenstein



Bureau at the Academy meeting in Menton 2016:
O. Eisenstein, M. Dupuis, J. Michl, H. Nakatsuji, G. Scuseria



3.6 Annual Medal Winners and Citations

- 1967** **W. KOLOS (University of Warsaw, Poland)**
"for his work on small molecules studied by means of electronic computers"
- 1968** **R.D. LEVINE (Hebrew University, Jerusalem, Israel)**
"pour sa contribution a la theorie des reactions chimiques"
- 1969** **A. DALGARNO (Harvard University, Massachusetts, USA)**
"pour sa contribution a la theorie des forces intermoleculaires"
- 1970** **R. HOFFMANN (Cornell University, New York, USA)**
pour sa methode de calcul des fonctions d'onde moleculaires et pour ses etudes theoriques des reactions chimiques"
- 1971** **E.R. DAVIDSON (University of Washington, USA)**
"for his fundamental contribution to the theory and calculation of properties of small molecules"
- 1972** **J. JORTNER (Tel Aviv University, Israel)**
"for his work on non-radiative transitions"
- 1973** **K. JOHNSON (Massachusetts Institute of Technology USA)**
"pour avoir mis au point des methodes de perfectionnement pour le calcul de proprietes des grosses molecules et des solides"
- 1974** **W.H. MILLER (University of California at Berkeley, USA)**
"pour ses travaux sur la theories des collisions"
- 1975** **L. SALEM (University Paris-Sud, Orsay, France)**
"pour ses travaux sur les processus photochimiques et sur les mecanismes de reactions chimiques"
- 1976** **J. CIZEK (University of Waterloo, Ontario, Canada)**
for the introduction of mathematical methods of quantum field theory into quantum chemistry"

- 1977 S.D. PEYERIMHOFF (University of Bonn, Germany)**
"for her outstanding contribution to the theoretical study of the geometry, reactivity and spectroscopic properties of molecules using configuration interaction"
- 1978 K. MOROKUMA (Institute of Molecular Science, Okazaki, Japan)**
"for his outstanding contribution to the quantum-mechanical study of excited states, reaction paths and intermolecular interactions"
- 1980 O. GOSCINSKI (Uppsala University, Sweden)**
"for his fundamental theoretical work on intermolecular forces and on time-dependent phenomena using propagator methods"
R.E. WYATT (University of Austin, Texas, USA)
"for his fundamental contribution to theoretical chemical dynamics"
- 1981 B. SIMON (Princeton University and Caltech, Pasadena, California, USA)**
"for his fundamental contribution to the theory of the stability of many particle systems and for his application of the complex scaling method to the theory of the stability of many molecular scattering and resonance phenomena"
- 1982 P. PULAY (University of Arkansas, USA)**
"for the analytic gradient method"
- 1983 J. SIMONS (Salt Lake City, Utah, USA)**
"for his theoretical contribution to the understanding of the electronic structure and behaviour of atoms and molecules, particularly negative ions"
- 1984 J.M. ANDRE (Facultes Universitaires Notre-Dame de la Paix, Namur, Belgium)**
"for his important theoretical work for the understanding of the properties of polymers and their industrial applications"
- 1985 P.E.M. SIEGBAHN (University of Stockholm, Sweden)**
"for his contributions to the development of methods for large-scale configuration interaction"
- 1986 W. JORGENSEN (Purdue University, USA)**
"for his work on the structure of organic liquids and on molecular reaction in solution"
- 1987 B. JEZIORSKI (University of Warsaw, Poland)**
"for his outstanding contribution to the coupled cluster method and to the theory of intermolecular forces"
- 1988 G.S. EZRA (Cornell University, USA)**
"for his incisive contribution to semi-classical quantization and to the theory of non-rigid molecules"
- 1989 D.C. CLARY (University of Cambridge, UK)**
"for his contribution to the quantum theory of molecular collisions"
- 1991 A.D. BECKE (Queen's University, Kingston, Canada)**
"for unique advances in numerical methods in density functional theory as applied to molecules, and for important developments in the understanding of the exchange-correlation functional that enters density functional theory"
- 1993 E.A. CARTER (University of California at Los Angeles, USA)**
"for development of multiple time scale Hartree-Fock molecular dynamics for surface chemical reactions"
- 1994 B.A. HESS (University of Bonn, Germany)**
"for development of the spin-free no-pair hamiltonian with external field projectors and his pioneering work in its application, opening the way for relativistic ab initio calculations including electron correlation for molecules in ground and excited states"

- 1995 N. MAKRI (University of Illinois, USA)**
"for her development of rigorous quantum mechanical path integral methods and subsequent calculations for the spin-boson problem, the paradigm for describing chemical reactions in condensed phases"
- 1997 J. GAUSS (University of Mainz, Germany)**
"for formulating and implementing very general GIAO based MBPT and Coupled-cluster correlation methods for the highly accurate prediction of NMR chemical shifts in molecules"
- W. YANG (Duke University, North Carolina, USA)**
"for his numerous contributions to the density functional theory of molecular electronic structure, in particular the 'divide and conquer' approach he originated for dealing with very large molecules"
- 1998 M. HEAD-GORDON (University of California, Berkeley, USA)**
"for his contributions to linear scaling in quantum chemistry"
- 1999 W. KLOPPER (Utrecht University, The Netherlands)**
"for his contributions to explicitly correlated methodology and applications in quantum chemistry"
- 2000 D. MANOLOPOULOS (Oxford University, UK)**
"for his contributions to the Quantum Theory of Molecular Collisions and Chemical Reactions"
- 2001 P. JUNGWIRTH (Heyrovsky Institute of Physical Chemistry, Czech Republic)**
"for his developments in quantum molecular dynamics of large polyatomic systems and applications to photochemical processes, in particular clusters"
- 2002 G. STOCK (University of Frankfurt, Germany)**
"for his contributions to the theory of ultrafast molecular photodynamics and its time-resolved spectroscopy, as well as to a variety of mixed quantum-classical methods for molecular dynamics"
- 2003 M. NOOIJEN (University of Waterloo, Canada)**
"for his contributions to the many-body treatment of the electronic structure of molecules, particularly his use of double similarity transformations to generalize coupled-cluster methods for excited states"
- 2004 L. GAGLIARDI (University of Palermo, Italy)**
"for her innovative contributions to prediction and understanding of new inorganic molecules using quantum chemical methods"
- 2005 S. HAMMES-SCHIFFER (Pennsylvania State University, USA)**
"for her development of innovative theories of electron and proton dynamics with insightful applications to biological processes"
- 2006 W. LIU (Beijing University, PR China)**
"for his contributions to relativistic quantum chemistry, especially the development of the Beijing Density Functional (BDF) code, and his formulation of an exact quasirelativistic decoupling of the Dirac equation."
- 2007 FREDERICK R. MANBY (University of Bristol, UK)**
"for expanding the applicability range and improving the accuracy of correlated molecular electronic-structure methods by a combination of local and density-fitting techniques"
- 2008 SO HIRATA (University of Florida, USA)**
"for theory and algorithm developments in electron correlated methods for molecules and extended systems"
- 2009 MIHÁLY KÁLLAY (The Technical University of Budapest, Hungary)**

- "for his innovative and pioneering contribution to algorithmic development for generating and implementing highly accurate many-body formulations"*
- 2010 GARNET K.-L.CHAN, (Cornell University, USA)**
"for his outstanding contribution to the density matrix renormalization group theory of molecular systems"
- 2011 ANDREAS KÖHN (Johannes Gutenberg-Universität Mainz, Germany)**
"for his contributions to explicitly correlated and multi-reference coupled cluster theories"
- 2012 PAUL W AYERS (McMaster University, Canada)**
"for his outstanding contributions to density functional theory and chemical reactivity theory"
- 2013 TAKESHI YANAI (Institute for Molecular Science, Japan)**
"for his development of novel approaches to incorporate dynamical correlation into DMRG using canonical transformation theory"
- 2014 EDWARD F. VALEEV (Virginia Tech, USA)**
"for the development of robust and practical methods for the inclusion of explicit R12/F12 effects in electronic structure calculations to address the basis set error in high-level correlation methods"
- 2015 KATARZYNA PERNAL (Lodz University of Technology, Poland)**
"for her outstanding contribution to the density matrix functional theory"

3.7 Abstracts from 53 Annual Academy Meetings

International Academy of Quantum Molecular Science

1967

Date of 1st Meeting:

18th – 20th June

Place of Meeting:

Villa Maria Serena, Menton, France

Members Present:

Founder Members present were:
R Daudel (France), P O Löwdin (Sweden)
R G Parr (USA), J A Pople (UK & USA)
B Pullman (France)

New Members elected:

L de Broglie (France), H M McConnell (USA)
C A Coulson (UK), M Karplus (USA)
M Kotani (Japan), H C Longuet-Higgins (UK)
R S Mulliken (USA), L Pauling (USA)
A Pullman (France), C C J Roothaan (USA)
J C Slater (USA)

Annual Medal:

W. Kolos (University of Warsaw, Poland)
*"for his work on small molecules studied by means of
electronic computers"*

Special Note:

Three of the new Members elected were
Nobel Prize Winners:
L de Broglie (France)
R S Mulliken (USA)
L Pauling (USA)

M Francis Palermo (Mayor of Menton) and
M Domergue (Curator of the Villa Maria Serena)
proposed that this Splendid Villa should be the
Headquarters of the Academy. M Palermo was
named "Benefactor" and M Domergue was
named "Archivist"

The Founding Members determined the Statues
of the Academy.

The Founding Members formed the Governing
Body of the Academy, with R Daudel as
President.

The declared intention was to further the
development of the field of Quantum Molecular
Science by, for example:
(1) Exchange of information on big computer
programmes
(2) Exchange of information on international
meetings
(3) Award of a prize to a brilliant young
scientist, who has carried out important research
within the field.

International Academy of Quantum Molecular Science

1968

Date of 2nd Meeting: 7th – 8th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: Not available

In the Chair: R Daudel (President)

New Members elected: J O Hirschfelder (USA)
E Hückel (Germany)
R Pauncz (Israel)
J H Van Vleck (USA)
E B Wilson (USA)

Annual Medal awarded to: R D Levine (Hebrew University, Jerusalem, Israel)
"pour sa contribution a la theorie des reactions chimiques"

Special Note: There was obviously much discussion on membership etc.
Benefactor Members (Membre Bienfaiteur) were proposed.
There was an Archivist (M Domergue in 1970).
There were three insignia which could be worn: in gold with six sapphires, in gold with three diamond roses for the President, The Vice President and Honorary Presidents, and a small insignia in gold. The Annual Medallists should receive a commemorative medal.

International Academy of Quantum Molecular Science

1969

Date of 3rd Meeting:	26 th – 27 th April
Place of Meeting:	Evergreen House, Baltimore, MD, USA
Members Present:	11 R Daudel, J O Hirschfelder, M Kotani, R S Mulliken, R G Parr, J A Pople, B Pullman, J C Slater, J H Van Vleck, E B Wilson, R Daudel (President in the Chair)
New Members elected:	S F Boys (UK); H Eyring (USA) F Hund (Germany); J Koutecky (Czechoslovakia)
Annual Medal:	A Dalgarno (Harvard University, USA) <i>"pour sa contribution a la theorie des forces intermoleculaires"</i>
Special Note:	<p>The Academy possessed a Statute of International Association. The French Government decided to underwrite the expenses of the French Academy Members at this meeting. They also agreed to provide a small budget for the annual meetings of the Academy in France.</p> <p>It was agreed that the 4th Meeting (8th – 10th July 1969) should be reserved for scientific discussion. The subjects to be covered were: “All electron calculations” (J A Pople); “Spin label studies in biological systems” (H C McConnell); “Quantum Biochemistry and Pharmacology” (A Pullman); “Quantum Theory of Chemical Reactivity” (R Daudel)</p>
Date of 4th Meeting:	8 th , 9 th , 10 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Special Note:	Minutes not available. It was a scientific meeting, outlined at earlier meetings. 8 July: Wavefunction calculations with all electrons (J A Pople). Lunch hosted by the Mayor of Menton. Spin labels in biological systems (H C McConnell) 9th July: Quantum theory of chemical reactivity (Daudel). Quantum biochemistry and pharmacology (A Pullman). Dinner at l’Hacienda. 10th July: Visits to the Greek Villa Kerylos, Beaulieu sur Mer, the gardens of the Ephrussi de Rothschild Foundation. Reception at Villa Maria Serena.

International Academy of Quantum Molecular Science

1970

Date of 5th Meeting: 8th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 9

R Daudel, M Karplus, J Koutecky,
P O Löwdin, R S Mulliken, R G Parr,
J A Pople, A Pullman, B Pullman

In the Chair: R Daudel (President)

New Members elected: W Heitler (Switzerland)
K Fukui (Japan)

Annual Medal: R Hoffmann (Cornell University, New York, USA)
*"pour sa methode de calcul des fonctions d'onde
moleculaires et pour ses etudes theoriques des reactions
chimiques"*

Special Note: At lunch, the 1969 medal was presented to A Dalgarno. Afterwards the 1970 medal was presented to R Hoffmann, who then delivered a lecture to the Academy.

International Academy of Quantum Molecular Science

1971

Date of 6th Meeting:	July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	8 R Daudel, J O Hirschfelder, M Karplus, J Koutecky, R G Parr, J A Pople, A Pullman, B Pullman
In the Chair:	R Daudel (President)
New Members elected:	E Scrocco (Italy)
Annual Medal awarded to:	E R Davidson (University of Washington, USA) <i>"for his fundamental contribution to the theory and calculation of properties of small molecules"</i>
Special Note:	At this meeting it was decided to organize the First International Congress in Quantum Chemistry, to be held July 1973, on the occasion of the 50 th Anniversary of Wave Mechanics. The Scientific Committee was the entire Academy, the organization Committee proposed was Coulson, Daudel , Fukui, Hirschfelder, Koutecky, Löwdin, Parr, Pauncz, Pople, A Pullman, B Pullman and Scrocco. The French Members formed the Executive Committee. Five mornings were dedicated to the symposium, with two or three lectures and one hour for discussion.

International Academy of Quantum Molecular Science

1972

Date of 7th Meeting:	July
Place of Meeting:	Villa Maria Serena, Menton, France
In the Chair:	R Daudel (President)
New Members elected:	V Fock (USSR)
Annual Medal awarded to:	J. Jortner (Tel Aviv University, Israel) <i>"for his work on non-radiative transitions"</i>
Special Note:	The Minutes do not tell us who was present at this meeting

International Academy of Quantum Molecular Science

1973

Date of 8th Meeting: 7th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 15

R Daudel, K Fukui, M Karplus,
J Koutecky, P O Löwdin, R S Mulliken,
R G Parr, R Pauncz, J A Pople,
A Pullman, B Pullman, E Scrocco,
J C Slater, J H Van Vleck, E B Wilson,

In the Chair: R Daudel (President)

New Members elected: G Herzberg (Canada)
K Ruedenberg (USA)
R McWeeny (UK)

Annual Medal awarded to: K. Johnson (Massachusetts Institute of
Technology USA
*"pour avoir mis au point des methodes de
perfectionnement pour le calcul de proprietes des grosses
molecules et des solides"*

Special Note: The Academy warmly thanked the Mayor of
Menton for all his organization towards the First
Congress.

The new Bureau consisted of:
B Pullman (President)
R G Parr (Vice-President)
J A Pople (Secretary)
R Pauncz (Treasurer)
R Daudel



Academy session in the Villa Maria Serena 1973
 (left to right) R G Parr, J H van Vleck, J C Slater, B Pullman, A Pullman, E Scrocco, R S Mulliken, R Daudel, E B Wilson, M Karplus, P-O Löwdin, J A Pople, R Pauncz, J Koutecky, K Fukui

International Academy of Quantum Molecular Science

1974

Date of 9th Meeting:	11 th – 12 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	9 R Daudel, J Koutecky, R G Parr, R Pauncz, J A Pople, A Pullman, B Pullman, K Ruedenberg, E Scrocco
In the Chair:	B Pullman (President)
New Members elected:	R Gaspar (Hungary) G G Hall (UK) C Sandorfy (Canada)
Annual Medal:	W H Miller (University of California at Berkeley, USA) <i>"pour ses travaux sur la theories des collisions"</i>
Mini Symposium presentations by:	J Koutecky: "Connection between the Resolvent Method and the Coulson-Longuet-Higgins formalism" R Pauncz: "Inter-relations between different types of construction of spin functions" R G Parr: "Can Ionization Potentials be computed from correlated wave functions?"

International Academy of Quantum Molecular Science

1975

Date of 10th Meeting:	15 th – 16 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	12 R Daudel, K Fukui, R Gaspar, G G Hall, M Karplus, J Koutecky, R McWeeny, R G Parr, A Pullman, B Pullman, C Sandorfy, E Scrocco
In the Chair:	B Pullman (President)
New Members elected:	A Davydov (USSR) H Hartmann (Germany)
Annual Medal:	L Salem (University Paris-Sud, Orsay, France) <i>"pour ses travaux sur les processus photochimiques et sur les mecanismes de reactions chimiques"</i>
Mini Symposium presentations by:	G G Hall: <i>"Reaction paths in solution"</i> R McWeeny: <i>"Excited states"</i> R Gaspar: <i>"Pseudopotentials"</i> A Pullman: <i>"Electrostatic molecular potentials"</i> R G Parr: <i>"Localisation and Electronegativity"</i> C Sandorfy: <i>"Hydrogen Bonds and Anesthesia"</i>
Special Note:	The participants were guests of M. Palermo, the Senator-Mayor of Menton, at a Dinner at the Villa Maria Serena

International Academy of Quantum Molecular Science

1976

Date of 11th Meeting:	24 th April
Place of Meeting:	New Orleans, Louisiana, USA
Members Present:	14 K Fukui, G G Hall, H Hartmann, M Karplus, J Koutecky, R McWeeny, R G Parr, A Pullman, B Pullman, K Ruedenberg, J H Van Vleck, P O Löwdin, R S Mulliken, J A Pople
In the Chair:	B Pullman (President)
New Members elected:	M Simonetta (Italy) E Heilbronner (Switzerland)
Annual Medal:	J. Cizek (University of Waterloo, Ontario, Canada) <i>"for the introduction of mathematical methods of quantum field theory into quantum chemistry"</i>
Special Note:	It was voted that members become senior members at age 65
Date of 12th Meeting:	10 th – 11 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	6 R Daudel, J A Pople, A Pullman, B Pullman, E Scrocco, M Simonetta
In the Chair:	B Pullman (President)
Special Note:	The new bureau was elected for 1976-79: B Pullman (President) R G Parr (Vice President) J A Pople (Secretary) R Pauncz (Treasurer) R Daudel

International Academy of Quantum Molecular Science

1977

Date of 13th Meeting: 12th – 13th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present:

In the Chair:

New Members elected: D P Craig (Australia)

Annual Medal awarded to: S.D. Peyerimhoff (University of Bonn, Germany)
*"for her outstanding contribution to the theoretical study of
the geometry, reactivity and spectroscopic properties of
molecules using configuration interaction"*

Special Note:

International Academy of Quantum Molecular Science

1978

Date of 14th Meeting: 11th – 12th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 8

R Daudel, K Fukui, M Karplus,
R G Parr, J A Pople, A Pullman,
B Pullman, M Simonetta

In the Chair: B Pullman (President)

New Members elected: R Hoffmann (USA)

Annual Medal awarded to: K. Morokuma (Institute of Molecular Science,
Okazaki, Japan)
"for his outstanding contribution to the quantum-mechanical study of excited states, reaction paths and intermolecular interactions"

Special Note: It was decided that proposals for membership or for the medal should be accompanied by one or two pages of argumentation or documentation for distribution to the entire membership. No later than six weeks before the meeting, the names and supporting documentation shall be sent to all members. Members are then asked to communicate their views.

International Academy of Quantum Molecular Science

1979

Date of 15th Meeting:	11 th – 12 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	5 R Daudel, M Kotani, J Koutecky, A Pullman, B Pullman
In the Chair:	B Pullman (President)
Special Note:	The new bureau for 1979-1982 was constituted: P O Löwdin (President) A Pullman (Vice President) K Fukui (Secretary) J Koutecky (Treasurer) R G Parr
Date of 16th Meeting:	30 th October
Place of Meeting:	Miyako Hotel, Keage, Kyoto, Japan
Members Present:	11 D P Craig, K Fukui, M Kotani, J Koutecky, P O Löwdin, R G Parr, J A Pople, A Pullman, B Pullman, K Ruedenberg, M Simonetta
In the Chair:	P O Löwdin (President)
New Members elected:	S Nagakura (Japan) E Teller (USA)
Annual Medal:	Not awarded

International Academy of Quantum Molecular Science

1980

Date of 17th Meeting:	9 th – 11 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	7 R Daudel, K Fukui, P O Löwdin, A Pullman, B Pullman, C Sandorfy and M Simonetta
In the Chair:	P O Löwdin (President)
Members' deceased since 1979 Meeting:	E Hückel
New Members elected:	W Lipscomb (USA)
Annual Medal awarded to:	1979 O. Goscinski (Uppsala University, Sweden) <i>"for his fundamental theoretical work on intermolecular forces and on time-dependent phenomena using propagator methods"</i> 1980 R.E. Wyatt (University of Austin, Texas, USA) <i>"for his fundamental contribution to theoretical chemical dynamics"</i>
Minisymposiums	A minisymposium on "Quantum Molecular Sciences: perspectives and Impact" was held, with contributions from K Fukui, C Sandorfy, B Pullman and P O Löwdin.
Special Note:	There was much discussion on the future direction of the Academy. In particular it was stressed that the Academy, as an International Body should try to obtain as broad a geographical background as possible, with scientific excellence remaining the main criterion for membership. The rigour of the election procedures was emphasized.

International Academy of Quantum Molecular Science

1981

Date of 18th Meeting:	8 th – 10 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	8 R Daudel, M Karplus, R J Koutecky, P O Löwdin, R G Parr, A Pullman, B Pullman, M Simonetta,
In the Chair:	P O Löwdin (President)
Members' deceased since 1980 Meeting:	J H Van Vleck
New Members elected:	E R Davidson (USA) A-C Tang (China)
Annual Medal awarded to:	B. Simon (Princeton University and Caltech, Pasadena, California, USA) <i>"for his fundamental contribution to the theory of the stability of many particle systems and for his application of the complex scaling method to the theory of the stability of many molecular scattering and resonance phenomena"</i>
Mini Symposium presentations by:	J. Koutecky: <i>"Correlation Effects in Li-Clusters"</i> P O Löwdin: <i>"Partitioning Technique, Perturbation Theory and Rational Approximations"</i> R G Parr: <i>"Circulant Orbitals"</i> B Pullman: <i>"Polymorphism of nucleic Acids and Chemical Carcinogenesis"</i> M Simonetta: <i>"The Interaction of Organic Molecules with Surfaces"</i>
Statutes:	It was agreed to put to the Membership the proposal that the number of Members allowed who are 65 years and under should be increased from 25 to 30.
Special Note:	It was agreed that the Academy should open a bank account, in Gainesville, Florida.

International Academy of Quantum Molecular Science

1982

Date of 19th Meeting:	13 th – 16 th June
Place of Meeting:	“Stenhusset,” The Royal Academy of Arts and Sciences, Uppsala, Sweden.
Members Present:	16 E R Davidson, R Daudel, K Fukui, R Gaspar, J Koutecky, R McWeeny P O Löwdin, R G Parr, A Pullman, B Pullman, R Pauncz, K Ruedenberg, C Sandorfy, M Simonetta, A C Tang, E B Wilson
In the Chair:	P O Löwdin (President)
New Members elected:	J Jortner (Israel) J Linderberg (Denmark) L Salem (France) R Zahradnik (Czechoslovakia)
Annual Medal awarded to:	P Pulay (University of Arkansas, USA) <i>"for the analytic gradient method"</i>
Statutes:	The proposal to increase the number of Members under 65 years from 25 to 30 was accepted
Special Note:	Up to this date, members under 65 years were known as ‘Ordinary Members’ and those above 65 years were known as ‘Senior Members’ There was a special meeting of the Academy on June 18th to discuss the 5th ICQC in 1985. It was decided to ask C Sandorfy to organise this event in Canada.

International Academy of Quantum Molecular Science

1983

Date of 20th Meeting: 10th – 13th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 9

R Daudel, G G Hall, M Kotani,
J Linderberg, P O Löwdin,
R G Parr, A Pullman, B Pullman,
M Simonetta,

In the Chair: P O Löwdin (President)

New Members elected: I Fischer-Hjalmars (Sweden)

Annual Medal awarded to: J. Simons (Salt Lake City, Utah, USA)
*"for his theoretical contribution to the understanding of
the electronic structure and behaviour of atoms and
molecules, particularly negative ions"*

Special Note: P O Löwdin reported that the plenary lectures of
the 1982 ICQC, were published by Reidel in
1983, and that the first four issues of IJQC 1983
contained the contributed papers (1700 pages)

International Academy of Quantum Molecular Science

1984

Date of 21st Meeting:	21 – 24 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	11 R Daudel, G G Hall, J Jortner, J Koutecky, P O Löwdin, S Nagakura, R G Parr, A Pullman, B Pullman, C Sandorfy, M Simonetta
In the Chair:	P O Löwdin (President)
New Members elected:	J. Paldus (Canada) H F Schaefer (USA)
Annual Medal awarded to:	J M André (Facultes Universitaires Notre-Dame de la Paix, Namur, Belgium) <i>"for his important theoretical work for the understanding of the properties of polymers and their industrial applications"</i>
Mini Symposium presentations by:	R Daudel: <i>(A new look on quantum chemistry)</i> G Hall: <i>(A simple model for a reaction surface)</i> J Jortner: <i>(Electron transfer and atom transfer in biophysical systems)</i> J Koutecky: <i>(Specific properties of the electronic structure of small molecules)</i> P O Löwdin: <i>(Approximate calculation of life-times of resonance states in the continuum from real stabilization graphs)</i> R G Parr: <i>(Density Functional Approach to the frontier electron theory of chemical reactivity)</i> A. Pullman: <i>(Quantum mechanical methodology for very large molecules: an application to problems of cation transport through membranes)</i> B Pullman: <i>Recognitory DNA-ligand interactions)</i> C Sandorfy: <i>(Rydberg states of transition metal complexes)</i> M Simonetta: <i>(The bridged (10)-annulene- bisenocaradiene equilibrium)</i>
Special Note:	The Academy decided to offer the proceedings of the 5 th ICQC (Montreal, 1985) to the International Journal of Quantum Chemistry.
R Daudel reported that a World Federation of Theoretical Organic Chemists had been established.	

International Academy of Quantum Molecular Science

1985

Date of 22nd Meeting:	18 th August
Place of Meeting:	University of Montreal, Montreal, Canada
Members Present:	20 E R Davidson, R Gaspar, G G Hall, G Herzberg, J Hirschfelder, R Hoffmann, J Jortner, J Linderberg, P O Löwdin, J Paldus, R G Parr, R Pauncz, J A Pople, A Pullman, B Pullman, C Sandorfy, M Simonetta, K Ruedenberg, A C Tang, R Zahradnik
In the Chair:	P O Löwdin Löwdin (President)
New Members elected:	D R Bates (UK) A D Buckingham (UK) W H Miller (USA) K Morokuma (Japan) I Shavitt (USA)
Annual Medal awarded to:	P.E.M. SIEGBAHN (University of Stockholm, Sweden) <i>"for his contributions to the development of methods for large-scale configuration interaction"</i>
Special Note:	Guidelines were approved for the organisation of International Congresses of Quantum Chemistry

International Academy of Quantum Molecular Science

1986

Date of 23rd Meeting: 10-12th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 13

E R Davidson, G G Hall, R Hoffmann,
J Jortner, J Koutecky, J Linderberg,
R McWeeny, R Pauncz, J A Pople,
A Pullman, B Pullman, L Salem,
C Sandorfy,

In the Chair: A Pullman (President)

Members deceased since 1985 Meeting: M Simonetta

New Members elected: W A Goddard (USA)
S D Peyerimhoff (Federal Republic of
Germany)

Annual Medal awarded to: W L Jorgensen (Purdue University, USA)
*"for his work on the structure of organic liquids and on
molecular reaction in solution"*

Mini Symposium presentations by:

E R Davidson: (e,2e) spectroscopy
G G Hall: Diabatic energy surfaces
R Hoffmann: A theoretical and chemical view of
surface science: chemisorption and reaction of
acetylene
J Jortner: Large clusters
J Koutecky: Magic numbers in cluster size
J Linderberg: Transition probabilities in atom-
diatom collisions
B Pullman; aspects of DNA-ligand interactions
L Salem: Chirality forces
C D Sandorfy: The effect of anesthetics on H-
bonds in gramicidin A channels

International Academy of Quantum Molecular Science

1987

Date of 24th Meeting: 18th – 19th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 16

J Jortner, M. Kotani, J Koutecky,
J Linderberg, P O Löwdin, R McWeeny,
K Morokuma, J Paldus, R Pauncz,
S D Peyerimhoff, J A Pople, A Pullman,
B Pullman, L Salem, C Sandorfy,
R Zahradnik

In the Chair: A Pullman (President)

Members deceased since 1986 Meeting: L de Broglie (*Noble Prize Winner*)
R S Mulliken (*Noble Prize Winner*)

New Members elected: J Cizek (Canada)
R Levine (Israel)
R A Marcus (USA)
E E Nikitin (USSR)
A Veillard (France)
F A Matsen (USA)

Annual Medal awarded to: B Jeziorski (University of Warsaw, Poland)
"for his outstanding contribution to the coupled cluster method and to the theory of intermolecular forces"

Mini Symposium presentations by: J Koutecky, J Linderberg
P O Löwdin, R McWeeny
J Paldus, R Pauncz
R Zahradnik

Special Note: The Voting Procedures are fully explained in the Minutes of this meeting

The Vice-Mayor of Menton addressed the Academy, on its 20th anniversary, and he expressed the hope that the ties with Menton will remain and even be reinforced. The President replied, with thanks.

International Academy of Quantum Molecular Science

1988

Date of 25th Meeting: 21st August

Place of Meeting: Israel Academy of Sciences and Humanities,
Jerusalem, Israel.

Members Present: 24

D P Craig, E R Davidson, K Fukui,
G G Hall, R Hoffmann, J Jortner, M Karplus,
J Koutecky, P O Löwdin, R D Levine,
W H Miller, K Morokuma, J Paldus, R G Parr,
R Pauncz, S D Peyerimhoff, J A Pople,
A Pullman, B Pullman,
K Ruedenberg, L Salem, H F Schaefer,
I Shavitt, A Veillard

In the Chair: A Pullman

New Members elected: N C Handy (UK)
W Kolos (Poland)
J Michl (USA)

Annual Medal awarded to: G.S. Ezra (Cornell University, USA)
*"for his incisive contribution to semi-classical quantization
and to the theory of non-rigid molecules"*

Special Note: P Löwdin announced the opening of a new
Institute in Japan for K Fukui, who was heartily
congratulated by the Academy

International Academy of Quantum Molecular Science

1989

Date of 26th Meeting: 9th – 11th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 12

E R Davidson, R Daudel, N C Handy,
J Linderberg J Michl, R G Parr,
R Pauncz, J A Pople, A Pullman,
B Pullman, L Salem, A Veillard

In the Chair: A Pullman

New Members elected: M J K Dewar (USA)
L Radom (Australia)

Annual Medal awarded to: D C Clary (University of Cambridge, UK)
"for his contribution to the quantum theory of molecular collisions"

Special Note: The new Mayor of Menton agreed to honour the engagements of the city towards the Academy

A Financial problem arose because of the small number of registrations at the Jerusalem Congress (for circumstances outside the control of the Academy); The Academy benefited from a generous gift from the Rothschild Foundation, negotiated by B Pullman.

International Academy of Quantum Molecular Science

1990

Date of 27th Meeting:	23 rd June – 24 th June
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	14 A D Buckingham, J. Cizek, R. Daudel, N C Handy, J Koutecky, J E Linderberg, R G Parr, R Pauncz, S D Peyerimhoff, J A Pople B Pullman, A Pullman, L Salem, R Zahradnik
In the Chair:	A Pullman
Members deceased since 1989 Meeting:	J O Hirschfelder
New Members elected:	W Kutzelnigg (Germany) R Lefebvre (France) P Pulay (USA)
Annual Medal:	not awarded
Mini Symposium presentations by:	J. Cizek N C Handy J Linderberg R G Parr R Pauncz B Pullman

International Academy of Quantum Molecular Science

1991

Date of 28th Meeting: 30th June – 1st July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 36

A D Buckingham, J Cizek, R Daudel,
E R Davidson, I Fischer-Hjalmars,
W A Goddard, G G Hall, N C Handy,
R Hoffmann, J Jortner, M Karplus,
W Kolos, J Koutecky, W Kutzelnigg,
R Lefebvre, J Linderberg, P O Löwdin,
R A Marcus, R McWeeny, J Michl,
W H Miller, K Morokuma, E Nikitin,
R G Parr, R Pauncz, S D Peyerimhoff,
J A Pople, P Pulay, A Pullman,
B Pullman, L Radom, K Ruedenberg,
L Salem, I Shavitt, A Veillard, R Zahradnik

In the Chair: A Pullman (President)

New Members elected: R J Bartlett (USA), M Basilevsky (Russia),
B-O Roos (Sweden) and W Kohn (USA)

Annual Medal awarded to: A D Becke (Queen's University, Kingston,
Canada)
*"for unique advances in numerical methods in density
functional theory as applied to molecules, and for important
developments in the understanding of the exchange-
correlation functional that enters density functional theory"*

Special Note: This was the last Academy Meeting at which all
five Founding Members were present

This meeting coincided with the 7th ICQC also
held in Menton (organiser L Salem)

International Academy of Quantum Molecular Science

1992

Date of 29th Meeting:	11 th – 12 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	17 R. J. Bartlett, R. Daudel, E R Davidson K. Fukui, N C Handy, J. Jortner W. Kutzelnigg, R. Lefebvre, F. A. Matsen K Morokuma, R G Parr, S. Peyerimhoff J.A. Pople, P. Pulay, A. Pullman, B. Pullman R. Zahradnik
In the Chair:	R G Parr (President)
New Members elected:	M Kasha (USA) P Pyykkö (Finland) P v R Schleyer (USA)
Annual Medal:	not awarded
Statutes:	Article 5 was amended (and approved) to increase the limit on the number of members under 65 years to 35
Special Note:	An elegant banquet was held at the Villa Maria Serena, hosted by the Mayor of Menton. Raymond Daudel gave a speech on the history of the academy (this was its 25th anniversary) and presented the Mayor with a Japanese flowered cloisonné dish

International Academy of Quantum Molecular Science

1993

Date of 30th Meeting:	10 th -11 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	18 R J Bartlett, J. Cizek, R. Daudel, N C Handy, W Kutzelnigg, R Lefebvre, J E Linderberg, R McWeeny, K Morokuma, R G Parr, B Pullman, J Paldus, A Pullman, P Pyykkö, L Salem, C Sandorfy, P v R Schleyer, R Zahradnik
In the Chair:	R G Parr (President)
Members deceased since 1992 Meeting:	E B Wilson M Kotani A S Davydov
New Members elected:	R Ahlrichs (Germany) A Dalgarno (USA) J-C Lorquet (Belgium) H Nakatsuji (Japan)
Annual Medal awarded to:	E A Carter (University of California at Los Angeles, USA) <i>"for development of multiple time scale Hartree-Fock molecular dynamics for surface chemical reactions"</i>
Mini Symposium presentations by:	R J Bartlett N C Handy J Linderberg R Lefebvre J Paldus P Pyykkö L Salem P v R Schleyer
Special Note:	Following the meeting a gala banquet was hosted by the Mayor of Menton

International Academy of Quantum Molecular Science

1994

Date of 31st Meeting:	18 th -19 th June
Place of Meeting:	Palace of Culture, Prague, Czech Republic
Members Present:	37 R Ahlrichs, R Bartlett, M V Basilevsky, A D Buckingham, E R Davidson, G G Hall, N C Handy, R Hoffmann, J Jortner, M Kasha, W Kolos, J Koutecky, W Kutzelnigg, R Lefebvre, R D Levine, J E Linderberg,, P-O LöwdinLöwdin, R McWeeny, J Michl, W H Miller, K Morokuma, H Nakatsuji, J Paldus, R G Parr, R Pauncz, S Peyerimhoff, J A Pople, P Pulay, P Pyykkö, B O Roos, C C Roothaan, K Ruedenberg, C Sandorfy, I Shavitt, P v R Schleyer, A Veillard, R Zahradnik
In the Chair:	R G Parr (President)
Members deceased since 1993 Meeting:	Sir David Bates
New Members elected:	P Cársky (Czechoslovakia) E Clementi (Sardinia) E Heller (USA) J Light (USA) P E M Siegbahn (Sweden)
Annual Medal awarded to:	B A Hess (University of Bonn, Germany) <i>"for development of the spin-free no-pair hamiltonian with external field projectors and his pioneering work in its application, opening the way for relativistic ab initio calculations including electron correlation for molecules in ground and excited states"</i>
Special Note:	The founding Members provided a sufficient sum for the support of the Annual Medal in perpetuity. A gala evening was hosted by R Zahradnik, which was attended by the Lord Mayor of Prague

International Academy of Quantum Molecular Science

1995

Date of 32nd Meeting: 8th – 9th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 21

R J Bartlett, M V Basilevsky, P Cársky, J Cizek,
R Daudel, E R Davidson, N C Handy, J Jortner,
W Kolos, W Kutzelnigg, K Morokuma, ,
H Nakatsuji, R G Parr, R Pauncz, J A Pople,
P Pulay, A Pullman, B Pullman, P Pyykkö,
C C J Roothaan, P v R Schleyer

In the Chair: R G Parr (President)

Members deceased since 1994 Meeting: Linus Pauling

New Members elected: W Meyer (Germany)
M Parrinello (Germany)

Annual Medal awarded to: N Makri (University of Illinois, USA)
*"for her development of rigorous quantum mechanical path
integral methods and subsequent calculations for the spin-
boson problem, the paradigm for describing chemical
reactions in condensed phases"*

Mini Symposium presentations by: M Basilevsky
P Cársky
J Cizek
K Morokuma
H Nakatsuji
R Pauncz
P Pulay
P Pyykkö

Special Note: The President will write to F Hund with
congratulations for his 100 year.

The Mayor of Menton entertained members and
their spouses to dinner at the Villa Maria Serena.

International Academy of Quantum Molecular Science

1996

Date of 33rd Meeting:	6 th - 7 th July
Place of Meeting:	Villa Maria Serena, Menton, France
Members Present:	14 R. J. Bartlett, E. Clementi, E R Davidson, N C Handy, R. Lefebvre, W. Meyer J. Michl, K Morokuma, H. Nakatsuji, R G Parr, A. Pullman, C.C.J. Roothaan, L. Salem, C. Sándorfy
In the Chair:	R G Parr (President)
Members deceased since 1995 Meeting:	B Pullman W Kolos
New Members elected:	W C Nieuwpoort (The Netherlands)
Annual Medal:	No medal awarded
Mini Symposium presentations by:	E Clementi J Michl C C J Roothaan R G Parr L Salem
Special Note:	<p>A postal ballot on the proposal to increase the number of academy members under 65 years from 37 to 37 did not receive the necessary support.</p> <p>The Mayor of Menton entertained members and their spouses to dinner at the Villa Maria Serena.</p>

International Academy of Quantum Molecular Science

1997

Date of 34th Meeting:	8 th – 9 th June
Place of Meeting:	Emory Conference Center, Hotel, Atlanta, Georgia, USA.
Members Present:	36 R. Ahlrichs, R. J. Bartlett, A. D. Buckingham, P. Cársky, J. Cizek E. Clementi, E R Davidson, W. A. Goddard, N C Handy, E. J. Heller, W. Kohn, J. Koutecky, W. Kutzelnigg, R. Lefebvre, J. C. Light, J-C Lorquet, W. Meyer, J. Michl, W. H. Miller, K Morokuma, H. Nakatsuji, W. C. Nieuwpoort R G Parr, S. Peyerimhoff, J. A. Pople, P. Pulay, A. Pullman, P. Pyykkö B. O. Roos C.C.J. Roothaan, K. Ruedenberg C. Sándorfy, H. F. Schaefer, P. v R. Schleyer, I. Shavitt, P. E. M. Siegbahn
In the Chair:	R G Parr (President)
Members deceased since 1996 Meeting:	F Hund
New Members elected:	A van der Avoird (The Netherlands) D Mukherjee (India)
Annual Medal:	J. Gauss (University of Mainz, Germany) <i>"for formulating and implementing very general GIAO based MBPT and Coupled-cluster correlation methods for the highly accurate prediction of NMR chemical shifts in molecules"</i> W. Yang (Duke University, North Carolina, USA) <i>"for his numerous contributions to the density functional theory of molecular electronic structure, in particular the 'divide and conquer' approach he originated for dealing with very large molecules"</i>
Special Note:	Emory University gave hospitality to the Academy

International Academy of Quantum Molecular Science

1998

Date of 35th Meeting: 4th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 23

P Cársky, E Clementi, E R Davidson
G Hall, N C Handy, W Kutzelnigg,
R Lefebvre, J Linderberg, R McWeeny
J Michl, W H Miller, D Mukherjee
H Nakatsuji, W C Nieuwpoort
M Parrinello, R Pauncz, L Radom
S Peyerimhoff, J A Pople, A Pullman,
B O Roos, C C.J Roothaan, L Salem

In the Chair: J A Pople (President)

Members deceased since 1997 Meeting: M J K Dewar
K Fukui

New Members elected: L Cederbaum (Germany)
D C Clary (UK)

Annual Medal: M Head-Gordon (University of California,
Berkeley, USA) (USA)
"for his contributions to linear scaling in quantum chemistry"

Special Note: It was agreed to establish a web page for the Academy.
The Mayor of Menton entertained Members and partners to a splendid banquet at the Villa Maria Serena

International Academy of Quantum Molecular Science

1999

Date of 36th Meeting: 10th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 16

R J Bartlett, P Cársky, L S Cederbaum,
D C Clary, N C Handy, W Kutzelnigg,
J-C Lorquet, D Mukherjee, W C Nieuwpoort
R G Parr, P Pulay, A Pullman,
S Peyerimhoff, B O Roos,
C C J Roothaan, A van der Avoird

In the Chair: S. Peyerimhoff (Vice-President)

Member deceased since 1998 Meeting: G. Herzberg

New Members elected: E-J Baerends (The Netherlands)
B Jeziorski (Poland)
J Tomasi (Italy)

Annual Medal: W. Klopper (Utrecht University, The Netherlands)
"for his contributions to explicitly correlated methodology and applications in quantum chemistry"

Special Note: The Mayor of Menton entertained Members and their partners to a splendid banquet at the Villa Maria Serena

The Academy congratulated the President, J A Pople, and W Kohn for their award of the 1998 Nobel Prize for Chemistry. R G Parr proposed the toast to them.

International Academy of Quantum Molecular Science

2000

Date of 37th Meeting:

4th – 5th June

Place of Meeting:

Villa Maria Serena, Menton, France

Members Present:

35

E-J Baerends, R J Bartlett, A D Buckingham,
P Cársky, L S Cederbaum, J Cizek
D C Clary, E Clementi, E R Davidson
N C Handy, B Jeziorski, J Koutecky,
W Kutzelnigg, R Lefebvre, J C Light
J-C Lorquet, W Meyer, W H Miller,
K Morokuma, D Mukherjee, H Nakatsuji,
W C Nieuwpoort, J Paldus, R G Parr,
R Pauncz, J A Pople, P Pulay,
P Pyykkö, S Peyerimhoff, L Radom,
B O Roos, C C J Roothaan, P E M Siegbahn,
J Tomasi, A van der Avoird

In the Chair:

J A Pople (President)

New Members elected:

A Becke (Canada)
R Kosloff (Israel)
J-P Malrieu (France)
M A Robb (UK)
J Tully (USA)

Annual Medal:

D Manolopoulos (Oxford University, UK)
*"for his contributions to the Quantum Theory of Molecular
Collisions and Chemical Reactions"*

Special Note:

The appointment of a new Bureau for the years
2000-2003 was made. Elected President:
K Morokuma, Vice-President: S. Peyerimhoff,
Treasurer: B O Roos, Secretary: W H Miller, and
Bureau Member: A Pullman.

Thanks were expressed for the work undertaken
by the retiring President (J A Pople) and
Secretary (N C Handy)

The Mayor of Menton entertained Members
and their partners to a splendid banquet at the
Villa Maria Serena

International Academy of Quantum Molecular Science

2001

Date of 38th Meeting: 7th – 8th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 23

P Cársky, D C Clary, E Clementi,
R Kosloff, W Kutzelnigg, R Lefebvre,
J-C Lorquet, W Meyer, H Nakatsuji,
W C Nieuwpoort, R G Parr, R Pauncz,
J A Pople, P Pulay, M A Robb,
C Sandorfy, P E M Siegbahn, J Tomasi,
K Morokuma, S Peyerimhoff, B O Roos,
W H Miller, A Pullman

In the Chair: K Morokuma (President)

Members deceased since 2000 Meeting: P-O Löwdin

New Members elected: G Schatz (USA)
H-J Werner (Germany)

Annual Medal: J Jungwirth (Heyrovsky Institute of Physical
Chemistry, Czech Republic)
"for his developments in quantum molecular
dynamics of large polyatomic systems and
applications to photochemical processes, in
particular clusters"

Mini Symposium presentations by: P Pulay: *'Ab initio theory, overview of present status and
future challenges'*
R G Parr: *'Perspectives on DFT, especially "atoms in
molecules" and future challenges'*
MA Robb: *'Issues related to combining dynamics and
quantum chemistry, especially for electronic non-adiabatic
processes'*
P E M Siegbahn: *'Using hybrid DFT methods to
understand mechanisms of metallo-enzyme reactions'*
D C Clary: *'Quantum dynamics of chemical reactions'*
R Kosloff: *'Rigorous grid-based methods for carrying
out quantum dynamical calculations of molecular
processes'*

Special Note: It was agreed to put to a postal ballot proposals
for the revision of the Statutes which were a
tidying up exercise involving the number of
members under 65 years, the procedures for
election, the annual medal and the postal vote.

The Mayor's dinner was a splendid occasion.

International Academy of Quantum Molecular Science

2002

Date of 39th Meeting: 6th – 7th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 24

E-J Baerends, R J Bartlett, P Cársky,
E Clementi, W A Goddard, N C Handy,
B Jeziorski, W Kutzelnigg, J E Linderberg
J-C Lorquet, W Meyer, J Michl,
D Mukherjee, W C Nieuwpoort, J A Pople,
P Pyykkö, G C Schatz, J Tomasi,
J C Tully, H-J Werner, K Morokuma,
S Peyerimhoff, B O Roos, W H Miller.

In the Chair: K Morokuma (President)

New Members elected: J-M André (Belgium)
K Hirao (Japan)
J Olsen (Denmark)

Annual Medal: G. STOCK (University of Frankfurt, Germany)
*"for his contributions to the theory of ultrafast molecular
photodynamics and its time-resolved spectroscopy, as well
as to a variety of mixed quantum-classical methods for
molecular dynamics"*

Discussions: A Ab initio theory (Chair: S Peyerimhoff)
Contributors:
B Jeziorski, D Mukherjee, H-J Werner
B Density Functional Theory (Chair: B O Roos)
Contributors:
E-J Baerends, N C Handy
C Nuclear Dynamics (Chair: W H Miller)
Contributors
G C Schatz, J C Tully, W H Miller

International Academy of Quantum Molecular Science

2003

Date of 40th Meeting:

19th – 20th July

Place of Meeting:

Universitaetsclub Bonn, Germany

Members Present:

39

R Ahlrichs, J-M André, E-J Baerends
R J Bartlett, A D Buckingham,
P Cársky, L S Cederbaum, J Cizek,
E Clementi, G C Hall, N C Handy,
K Hirao, B Jeziorski, J Jortner,
W Kutzelnigg, J E Linderberg,
J-C Lorquet, W Meyer, J Michl,
W H Miller, K Morokuma,
D Mukherjee, H Nakatsuji,
W C Nieuwpoort, J Olsen, J Paldus,
R G Parr, R Pauncz, S Peyerimhoff,
J A Pople, P Pykkö, M A Robb,
B O Roos, C C J Roothaan,
G C Schatz, P E M Siegbahn,
P Pulay, J Tomasi, H-J Werner

In the Chair:

K Morokuma (President)

Members deceased since 2002 Meeting:

R Gaspár

New Members elected:

W Domcke (Germany)
K N Houk (USA)
J P Perdew (USA)
M A Ratner (USA)

Annual Medal:

M Nooijen (Princeton University, USA)
*"for his contributions to the many-body treatment of
the electronic structure of molecules, particularly his use
of double similarity transformations to generalize
coupled-cluster methods for excited states"*

Special Note:

There was an extensive discussion on how the Academy's modest resources might most wisely be used.

An enjoyable dinner was held at the Universitätsclub for members, their guests and various academic guests from the University of Bonn.

International Academy of Quantum Molecular Science

2004

Date of 41st Meeting: 3rd – 4th July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 26

J-M. André, P Cársky, J Cizek, E Clementi,
W Domcke, N C Handy, K Hirao, K Houk,
B Jeziorski, R Kosloff, W Kutzelnigg,
R Lefebvre, J E Linderberg, J C Lorquet,
W Meyer, J Michl, W H Miller, K Morokuma,
H Nakatsuji, W C Nieuwpoort, S Peyerimhoff,
P Pyykkö, B O Roos, C C J Roothaan,
K Ruedenberg, J Tomasi

In the Chair: K Morokuma (President)

Members deceased since 2003 Meeting: H C Longuet-Higgins
J A Pople
E Teller

New Members elected: M S Gordon (USA)
S Kato (Japan)

Annual Medal: Laura Gagliardi (University of Palermo)
*“for her innovative contributions to prediction and
understanding on new inorganic molecules using quantum
chemical methods”.*

Special Note: A comprehensive report on innovative teaching
promoting Theoretical Chemistry was discussed.

The improvement in the Academy's financial
position enabled a financial reward to be
attached to the Annual Medal, and also a
financial reward to be made for each of the five
best posters at each ICQC.

Research Reports were presented by: J Cizek,
J Michl, H Nakatsuji, B Roos, K Ruedenberg.

A very enjoyable dinner was held at the Villa
Maria Serena for members, their guests and
Menton city officials.

International Academy of Quantum Molecular Science

2005

Date of 42nd Meeting:

2nd – 3rd July

Place of Meeting:

Villa Maria Serena, Menton, France

Members Present:

28

J-M. André, E-J Baerends, P Cársky,
E Clementi, W Domcke, M S Gordon,
N C Handy, K Hirao, B Jeziorski,
S Kato, W Kutzelnigg, R Lefebvre,
J E Linderberg, J C Lorquet, W H Miller,
K Morokuma, H Nakatsuji, W C Nieuwpoort,
J Olsen, R Pauncz, J P Perdew, P Pyykkö,
M A Robb, B O Roos, C C J Roothaan,
K Ruedenberg, J Tomasi, J Tully

In the Chair:

K Morokuma (President)

New Members elected:

T U Helgaker (Norway)
M Dupuis (USA)

Annual Medal:

Sharon Hammes-Schiffer (Pennsylvania State University)

"for her development of innovative theories of electron and proton dynamics with insightful applications to biological processes"

Special Note:

Panel discussions were held to provide an overview of the present status on topics of interest.

(a) *Relativistic effects in quantum chemistry*
(Pyykkö, Hirao, Kutzelnigg, Baerends)

(b) *Electron Correlation* (Ross, Olsen, Nakatsuji)

(c) *Quantum Dynamics* (Miller, Tully, Domcke)

Mini Symposium

A mini symposium was held for high school students from Menton with presentations by Tomasi, Kutzelnigg, André, Pyykkö.

A very enjoyable dinner was held at the Villa Maria Serena for members, their guests and Menton city officials.

International Academy of Quantum Molecular Science

2006

- Date of 43rd Meeting:** 20th – 21st May
- Place of Meeting:** Kyoto TERRSA, Kyoto, Japan
- Members Present:** 36
- E-J Baerends, R J Bartlett, P Cársky,
L S Cederbaum, D C Clary, E Clementi,
E R Davidson, W Domcke, M Dupuis,
M S Gordon, N C Handy, T U Helgaker,
K Hirao, K N Houk, S Kato,
R Kosloff, W Kutzelnigg, J Michl,
W H Miller, K Morokuma, D Mukerjee,
H Nakatsuji, W C Nieuwpoort, J Paldus,
R G Parr, J P Perdew, S Peyerimhoff,
P Pulay, J P Pyykkö, L Radom,
M Ratner, C C J Roothaan, K Ruedenberg,
I Shavitt, P E M Siegbahn, H-J Werner
- In the Chair:** K Morokuma (President)
- Members deceased since 2005 Meeting:** J Koutecky
- New Members elected:** O Eisenstein (France)
M Head-Gordon (USA)
W A Lester (USA)
D G Truhlar (USA)
W Yang (USA)
- Annual Medal:** Wenjian Liu (Peking University, Beijing, China)
“for his contributions to relativistic quantum chemistry, especially the development of the Beijing Density Functional (BDF) code, and his formulation of an exact quasirelativistic decoupling of the Dirac equation.”
- Special Note:** Election of new officers: those elected were
President: S Peyerimhoff, Vice-President:
P Pyykkö, Secretary: K Hirao, Treasurer:
M Gordon, Fifth Member: R Bartlett
- It was agreed to put to a postal vote a proposal to eliminate Article 5 of the Statutes (this is the Article which restricts the number of members under 65 years to 35).
- An elegant dinner was held for members and their guests at the Saami Japanese restaurant.

International Academy of Quantum Molecular Science

2007

Date of 44th Meeting: 7 – 8 July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 32

J-M André, EJ Baerends, R Bartlett, P Cársky, J Cizek, E Clementi, M Dupuis, M Gordon, N Handy, T Helgaker, K Hirao, B Jeziorski, S Kato, W Kutzelnigg, R Lefebvre, WA Lester, R Levine, J E Linderberg, J-C Lorquet, W Meyer, J Michl, D Mukherjee, R Pauncz, S Peyerimhoff, P Pyykkö, B O Roos, M Robb, CCJ Roothaan, J Tomasi, A van der Avoird, H-J Werner, W Yang

In the Chair: S Peyerimhoff (President)

Members deceased since 2006 Meeting: Frederick A Matsen, Camille Sandorfy
Raymond Daudel, Edgar Heibronner

New Members elected: Walter Thiel (Germany), Tom Ziegler (Canada)

Annual Medal: Frederick Roy Manby (U. of Bristol,UK)
“for expanding the applicability range and improving the accuracy of correlated molecular electronic-structure methods by a combination of local and density fitting techniques”

Special Note: Article 5 of the IAQMS Statutes is eliminated, following a postal vote (Nov.2006-Jan.2007). Out of a total of 54 members 44 voted for elimination; i.e. a vote of two thirds of those responding was reached.

N C Handy presented abstracts of the Annual meetings 1967-2007 and outlines of the International Congresses. The president agreed to add an historical part of the Academy and to distribute the entire work as a booklet in 2008. Jan Linderberg presented the booklet “Inception of Quantum Chemistry at Uppsala” ed.A.Fröman and Jan Linderberg

A survey of the state of Quantum Molecular Science in different countries of the world was presented by the members. It was suggested to make a brochure of these data for distribution.

J-M André and J-C Lorquet (“Menton Committee”) reported on the “Conférence de Vulgarisation” held at the Villa Marina Serena on July 6 for the public of Menton.

International Academy of Quantum Molecular Science

2008

Date of 45th Meeting: 5 - 6 July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 21

J-M André, P Cársky, E Clementi, M Dupuis, J-C Lorquet, M Gordon, K Hirao, B Jeziorski, J Michl, W H Miller, K Morokuma, H Nakatsuji, W C Nieuwpoort, J Perdew, S Peyerimhoff, P Pyykkö, B O Roos, CCJ Roothaan, K Ruedenberg, J Tomasi, T Ziegler

In the Chair: S Peyerimhoff (President)

New Members elected: Vincenzo Barone (Italy), Shigeru Nagase (Japan), Zhigang Shuai (PR China), Miroslav Urban (Slovakia)

Annual Medal: So Hirata (U. of Florida, USA)
“for theory and algorithm development in electron correlated methods for molecules and extended systems”

Special Note: The Academy presented a Medal with the inscription *“Jean-Claude Guibal, Maire de Menton, en reconnaissance des services rendues à l’IAQMS, 2008”* to the Mayor. The ceremony took place at the impressive “salle du conseil” of the city hall of Menton. Guibal has supported our Academy as mayor of Menton since 1989. The Journal Nice Matin reported on the event.

The booklet “International Academy of Quantum Molecular Science: 40 Years 1967 – 2007” has been sent to all members in May 2008

The state of Quantum Molecular Science in countries throughout the world was commented on the basis of responding questionnaires. Possible ways to improve the visibility of the Academy were suggested, its situation with respect to age, gender and international representation by its members was discussed

J-M André, P Pyykkö and M Dupuis gave public lectures to the people of Menton.

A very enjoyable dinner was held at the Villa Maria Serena with Menton city officials and colleagues from the Lycée Pierre&Marie Curie.

International Academy of Quantum Molecular Science

2009

- Date of 46th Meeting:** 21 – 22 June
- Place of Meeting:** University main building, Helsinki, Finland
- Members Present:** 42
R Ahlrichs, J-M André, V Barone, R Bartlett, P Cársky, J Cizek, E Clementi, E. Davidson, W Domcke, O Eisenstein, M Gordon, G Hall, N Handy, T Helgaker, K Hirao, K Houk, B Jeziorski, R Kosloff, W Kutzelnigg, J Linderberg, W Meyer, J Michl, K Morokuma, D Mukherjee, H Nakatsuji, J Olsen, S Peyerimhoff, P Pulay, P Pyykkö, L Radom, M Robb, B Roos, K Ruedenberg, HF Schaefer, Z Shuai, P Siegbahn, W Thiel, J Tomasi, D Truhlar, M Urban, H-J Werner, T Ziegler
- In the Chair:** S Peyerimhoff (President)
- Members deceased since 2008 Meeting:** Inga Fischer-Hjalmars, Au-Chin Tang
- New Members elected:** Emily A. Carter (USA), Jürgen Gauss (Germany), Kwang S. Kim (Korea), Mel Levy (USA) Gustavo E. Scuseria (USA), John Stanton (USA)
- Annual Medal:** Mihaly Kallay (Technical University of Budapest, Hungary)
“for his innovative and pioneering contribution to algorithmic development for generating and implementing highly accurate many-body formulations
- Special Note:** A preliminary version of the Survey of QMS in the world containing information from 30 countries plus an extended Appendix of groups in the various countries had been distributed to all members in April. It is also on the Academy home page. Further steps to publicize and distribute this document will be considered later on.
- The Menton Committee suggests to give 2-days lectures to selected schools in Menton during the schoolyear, as suggested by Mr. Beauvais (coordinator in Menton), French speaking members are ready to do this
- Election of new Bureau: President: Pekka Pyykkö, Vice-President: Josef Michl, Secretary General: Kimihiko Hirao, Treasurer: Mark Gordon, Fifth Member: Jean-Marie André
- On Sunday evening members enjoyed a wonderful Cruise and Dinner.

International Academy of Quantum Molecular Science

2010

Date of 47th Meeting: 3 – 4 July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 34

J-M André, EJ Baerends, R Bartlett, P Cársky, M Dupuis, O Eisenstein, J Gauss, M Gordon, T Helgaker, K Hirao, B Jeziorski, K Kim, W Kutzelnigg, R Lefebvre, M Levy, J C Lorquet, W Meyer, J Michl, W Miller, W Nieuwpoort, R Parr, S Peyerimhoff, P Pyykkö, L Radom, M Robb, K Ruedenberg, H-F Schaefer, G Scuseria, J Stanton, J Tomasi, M Urban, A van der Avoird, H-J Werner, W Yang

In the Chair: Pekka Pyykkö (President)

Members deceased since 2009 Meeting: Björn Roos, Shigeaki Kato

New Members elected: William L. Jorgensen (USA), Nancy Makri (USA), Krishnan Raghavachari (USA), Krzysztof Szalewicz (USA)

Annual Medal: Garnet K.-L. Chan (Cornell University, USA)
“for his outstanding contribution to the density matrix renormalization group theory of molecular systems”

Special Note: Statistics about members with respect to age and countries are discussed. It is recommended that the number of nominations per member should be limited and members are asked for an internal ranking of their proposed candidates.

The “Menton Committee” reports that J-M André and J-C Lorquet have delivered talks at the Lycée Marie Curie in Menton and that the directors hope for the extension of such cooperation. A proposal is to create a “special prize of the Academy” to be awarded to an alumnus of the Lycée to undertake postgraduate studies in theoretical chemistry/molecular

The survey of the state of QMS in the world includes now 40 countries and the latest version (1.2.1) is on the Academy’s homepage.

A very enjoyable dinner was held on Saturday at the Villa Maria Serena for Academy members, their guests and Menton officials.

International Academy of Quantum Molecular Science

2011

Date of 48th Meeting: 2 – 3 July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 33

J-M André, P Cársky, E Clementi, W Domcke, M Dupuis, M Gordon, O Eisenstein, J Gauss, N Handy, T Helgaker, B Jeziorski, L Jorgensen, K Kim, W Kutzelnigg, R Lefebvre, WA Lester, J C Lorquet, N Makri, W Meyer, J Michl, D .Mukherjee, W Nieupoort, R Parr, S Peyerimhoff, P Pulay, P Pyykkö, L Radom, K Raghavachari, K Ruedenberg, G Scuseria, Z Shuai, K Szalewicz, W Thiel, M Urban

In the Chair: Pekka Pyykkö (President)

Members deceased since 2010 Meeting: Alberte Pullman, William Lipscomb

New Members elected: Jean-Luc Bredas (USA), Wim Klopper (Germany), H.B. (Berny) Schlegel (USA)

Annual Medal: Andreas Köhn (University Mainz, Germany))
“for his contributions to explicitly correlated and multi-reference coupled cluster theories

Special Note: Addition to the Minutes of the previous meeting:
the membership agreed to eliminate the cash prize that had been associated with the Academy Medal

K Raghavachari presented a summary of the status of QMS in India.

The distribution of members with respect to gender, nationality and research disciplines are discussed and needs more attention in nominations.

The lectures presented by French-speaking members of the Academy at the menton high school continue to be well received and will continue

The enjoyable dinner for members and their guest on Saturday evening at the Villa Maria Serena was joined by representatives of the Mayor of Menton

International Academy of Quantum Molecular Science

2012

Date of 49th Meeting:

24 – 25 June

Place of Meeting:

Ekeley Building, University of Colorado,
Boulder, USA

Members Present:

33

J-M André, EJ Baerends, R Bartlett, M Dupuis, O Eisenstein, J Gauss, M Gordon, K Hirao, K Houk, K Kim, W Klopper, W Lester, W Meyer, J Michl, WH Miller, K Morokuma, D Mukherjee, H Nakatsuji, W Nieuwpoort, P Pulay, K Raghavachari, M Ratner, K Ruedenberg, H B Schlegel, G Scuseria, J Stanton, Z Shuai, K Szalewicz, M Urban, A van der Avoird, H-J Werner, W Yang, T Ziegler

In the Chair:

Josef Michl (Vice-President)

Members deceased since 2011 Meeting: Eolo Scrocco

New Members elected:

Poul Jorgensen (Denmark), Georg Kresse (Austria), Frank Neese (Germany), Andreas Savin (France), Peter A Schwerdtfeger (New Zealand), Sheiichiro Ten-no (Japan)

Annual Medal:

Paul W. Ayers (Mamaster University, Canada)
“for his outstanding contributions to density functional theory and chemical reactivity theory”

Special Note:

The President was unable to attend the meeting due to health problems.
A proposal of Don Truhlar and fourteen other members to change the IAQMS Statutes in order to alter the election procedures for new members (annual e-mail or internet ballot) was thoroughly discussed. Among the members present there was a strong sentiment that face-to-face discussions at the meetings are very valuable. A committee of outgoing and the incoming Bureau was formed to reflect the comments made and to propose further action.

Election of new Bureau: President: Josef Michl, Vice-President: Gustavo Scuseria, Secretary General: Hiroshi Nakatsuji, Treasurer: Michael Dupuis, Fifth member: Odile Eisenstein

A very enjoyable dinner was held at the Red Lion Inn for Academy members and their guests.

International Academy of Quantum Molecular Science

2013

Date of 50th Meeting: 6 – 7 July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 36

J-M André, EJ Baerends, V Barone, P Cársky, E Clementi, M Dupuis, J Gauss, M Gordon, K Hirao, B Jeziorski, W Klopper, G Kresse, W Kutzelnigg, R Lefebvre, WA Lester, J E Linderberg, J C Lorquet, J-P Malrieu, W Meyer, J Michl, H Nakatsuji, F Neese, W Nieuwpoort, O Eisenstein, S Peyerimhoff, P Pulay, P Pyykkö, K Ruedenberg, A Savin, P Schwerdtfeger, E Scuseria, Z Shuai, W Thiel, J Tomasi, M Urban, H-J Werner

In the Chair: Josef Michl (President)

Members deceased since 2012 Meeting: Nicholas C. Handy, Isaiah Shavitt

New Members elected: Joel M. Bowman (USA), David M. Ceperley (USA), Stefan Grimme (Germany), David E. Manolopoulos (UK), Gregory Voth (USA)

Annual Medal: Takeshi Yanai (Institute for Molecular Science, Japan)
“for his development of novel approaches to incorporate dynamical correlation into DMRG using canonical transformation theory”

Special Note: The proposal of Truhlar and co-signers to introduce internet election of members did not get enough positive postal votes to pass

New members Kresse, Neese, Savin and Schwerdtfeger gave brief presentations on their recent interests and active discussion followed.

The Menton Committee is enlarged; members are J-M André, J-C Lorquet, A Savin and O Eisenstein.

A Canvassing committee is set up to deal with the underrepresentation of members with respect to gender, country and subdisciplines and to identify worthy individuals for membership.

On Saturday evening members enjoyed the Mayors dinner at the Villa Serena together with representatives of the Mayor and Madame Claudette Rebaudo, in charge of educational issues in Menton.

International Academy of Quantum Molecular Science

2014

Date of 51th Meeting:

5 – 6 July

Place of Meeting:

Villa Maria Serena, Menton, France

Members Present:

39

J-M André, EJ Baerends, R Bartlett, P Cársky, D Ceperly, E Clementi, M Dupuis, O Eisenstein, J Gauss, M Gordon, T Helgaker, K Hirao, B Jeziorski, W Klopper, G. Kresse, W Kutzelnigg, R Lefebvre, J C Lorquet, N Makri, W Meyer, J Michl, W Miller, D Manolopoulos, H Nakasutji, W Nieupoort, S Peyerimhoff, P Pyykkö, L Radom, A Savin, HS Schaefer, G Scuseria, Z Shuai, K Szalewicz, S Ten-no, J Tomasi, M Urban, G Voth, H-J Werner, T Ziegler

In the Chair:

Josef Michl (President)

New Members elected:

Millard Alexander (USA) Ria Broer-Braam (Netherlands), Garnet Kin-Lic Chan (USA), Sharon Hammes-Schiffer (USA), So Hirata (USA), Wenjian Liu (PR China), Benedetta Menucci (Italy), Josef Noga (Slovakia)

Annual Medal:

Edward F Valeev (Virginia Tech. Blacksburg, VA, USA)

“for the development of robust and practical methods for the inclusion of explicit R12/F12 effects in electronic structure calculations to address the basis set error in high-level correlation methods.”

Special Note:

The IAQMS congratulates Martin Karplus, Michael Levitt and Arie Warshal to the 2013 Nobel Prize in Chemistry.

New members Ceperley, Manolopoulos, Tenno, Voth gave brief presentations on their recent interests.

The Canvassing committee (G Scuseria, O Eisenstein, M Gordon) is extended to include K Hirao and D Mukherjee

The call by E Clementi for a more dynamic IAQMS was thoroughly discussed

The Mayor's dinner was joined by the First Deputy Mayor, Nicolas Antonietti, and guests.

International Academy of Quantum Molecular Science

2015

Date of 52nd Meeting:

7 – 8 June

Place of Meeting:

Tsinghua University, Beijing, China

Members Present:

49

M Alexander, J-M André, J Bowman, R Broer-Bram, P Cársky, G Chan, D Clary, E Clementi, M Dupuis, O Eisenstein, S Hammes-Schiffer, M Head-Gordon, T Helgaker, K Hirao, S Hirata, R Hoffmann, K Houk, B Jeziorski, P Jorgensen, K Kim, W Liu, N Makri, R Marcus, B Mennucci, W Miller, J Michl, K Morokuma, D Mukherjee, H Nakatsuji, W Nieuwpoort, J Noga, J Olsen, P Pulay, P Pyykkö, L Radom, K Raghavachari, A Savin, G Schatz, B Schlegel, P Schwerdtfeger, E Scuseria, Z Shuai, S Ten-no, W Thiel, D Truhlar, M Urban, A van der Avoird, H-J Werner, W Yang

In the Chair:

Josef Michl (President)

Members deceased since 2014 Meeting:

Alexander Dalgarno, Tom Ziegler, Paul von Ragué Schleyer, Harden M McConnell

New Members elected:

Thom H Dunning Jr (USA), Peter M.W. Gill (Australia), Anna Krylov (USA), Ursula Röthlisberger (Switzerland), Sason Shaik (Israel), Arieh Warshel (USA)

Annual Medal:

Katarzyna Pernal (Lodz University of Technology, Poland)

“for her outstanding contribution to the density matrix functional theory”

Special Note:

eight members of those elected 2013/14 gave brief presentations of their recent research interests.

Odile Eisenstein distributed guidelines for ICQC organizing procedures.

Patenting of quantum chemical methods and algorithms was discussed; the majority was against it.

A modification of the procedure for member election is proposed by the Bureau. It is a compromise so that those, not attending the annual meetings have more influence on the voting procedure. The final vote will remain at the annual meeting. The Canvassing Committee will be elected by secret ballot and serve for one year.

International Academy of Quantum Molecular Science

2016

Date of 53rd Meeting: 2 - 3 July

Place of Meeting: Villa Maria Serena, Menton, France

Members Present: 39

R Broer-Braam, R Bartlett, P Cársky, M Dupuis, O Eisenstein, P Gill, M Gordon, S Grimme, M Head-Gordon, T Helgaker, S Hirata, B Jeziorski, W Jorgensen, A Krylov, W Liu, J C Lorquet, N Makri, J-P Malrieu, B Mennucci, W Meyer, J Michl, H Nakatsuji, W Nieuwpoort, J Noga, S Peyerimhoff, P Pulay, P Pyykkö, L Radom, U Röthlisberger, K Ruedenberg, H Schaefer, P Schwerdtfeger, G Scuseria, S Shaik, K Scalewicz, S Ten-no, D Truhlar, M Urban, H-J Werner

In the Chair: Josef Michl (President)

Members deceased since 2015 Meeting: Walter Kohn, David P Craig

New Members elected: Ali Alavi (UK and Germany), Jiali Gao (USA), Marcel Nooijen (Canada), Julia Rice (USA) Trond Saue (Norway)

Annual Medal: The final vote was sufficiently split that none of the candidates reached the requirements for the award.

Special Note: four members elected 2015 gave brief presentations on their recent interests.

Activities for the celebration of the 50th anniversary of IAQMS in 2017 are discussed. J-M André, O Eisenstein, T Helgaker and S Peyerimhoff agreed to organize the various projects and events.

Anna Krylov was elected the chairperson of the new Canvassing Committee. The suggestion (R Bartlett) that the number of sponsors for a nomination for membership or medal be limited to four received full support.

On Saturday evening members and guest were invited to the Mayor's dinner at the Villa Maria Serena and were joined by representatives of the Mayor, Nicolas Antonietti and Pauline Foti.

3.8 Outline of the 15 International Congresses

THE FIRST INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

Place:	Menton, France
Date:	July 4-10, 1973
Scientific Committee:	All Members of the Academy
Organising Committee:	A Pullman, C A Coulson, R Daudel, K Fukui, J O Hirschfelder, J Koutecky, P O Löwdin, R G Parr, R Pauncz, J A Pople, B Pullman, E Scrocco
Executive Committee:	A Pullman, R Daudel, B Pullman
Morning Sessions:	(1) <i>Methods of Quantum Chemistry</i> (Löwdin, Slater, Davidson, Kolos) (2) <i>Electronic Structure and Conformation of Molecules</i> (Koutecky, Pople, B Pullman) (3) <i>General Theory of Chemical Reactivity</i> (Daudel, Karplus, Fukui) (4) <i>Formation and Evolution of Excited States</i> (Parr, Jortner and Mukamel, Heilbronner) (5) <i>Effects of Environment on Behaviour of Molecules</i> (A Pullman, Buckingham, Sinanoglu, Morokuma, Iwata and Lathan)
Afternoon Sessions:	(1) <i>Methods in Quantum Chemistry. Use of computers</i> (2) <i>Atomic and Molecular Spectroscopy</i> (3) <i>Electronic Structures & Properties of Chemical Species</i> (4) <i>Chemical reactions. Collisions. Reaction paths. Chemical equilibrium. Catalysis. Application of Quantum chemistry in Industry</i> (5) <i>Excitation and relaxation Processes. Photochemical reactions. Mass Spectroscopy.</i> (6) <i>Quantum Biochemistry and quantum pharmacology</i> (7) <i>Intermolecular forces, role of environment</i> (8) <i>Quantum chemistry and its relationships with the physics of liquids and solids</i>
Attendance:	400 persons from 40 countries
Opening Addressess:	Duc Louis de Broglie (in French) and Raymond Daudel (in French and English)
Publication:	“The World of Quantum Chemistry” Editors: R Daudel and B Pullman. Reidel (1973)
Comment:	For all those interested in the history of our subject, this is indeed a landmark meeting (NCH)

THE SECOND INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

- Place:** New Orleans, Louisiana, USA
- Date:** April 19th – 24th 1976
- Organising Committee:** R G Parr (Chairman), J A Pople, K. Ruedenberg
P Politzer (Local Organizer) with B Anex and R Flurry
- Congress:** Foundations of Quantum Chemistry
(K Ruedenberg, R McWeeny, R Daudel
and Y Ohrn)
Molecular Scattering
(J O Hirschfelder, W H Miller, R D Levine)
Quantum Organic Chemistry and Beyond
(B Pullman, G G Hall, A Pullman,
R E Christoffersen and R P Angelia)
Potential Surfaces, Transition States, and
Intermediates in Chemical and Photochemical
Processes
(M Karplus, S D Peyerimhoff, R J Buenker
and L Salem)
Surface Quantum Chemistry and Catalysis
(K Fukui, J Koutecky, J R Schrieffer and
K H Johnson)
- Sponsorship:** Financial support was received from:
National Science Foundation, Petroleum Research Fund, United
States Air Force and Hewlett-Packard Corporation
- Opening Address:** by B Pullman, who said ‘...Aims of the Academy were to
stimulate contacts, collaboration and friendship between
quantum molecular scientists at the International level ...’
- Publication:** Plenary Lectures published by Reidel in 1976, as
*“New World of Quantum Chemistry, Proceedings of the Second
International Congress of Quantum Chemistry”*, eds B Pullman
and R G Parr

THE THIRD INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

Place:	Kyoto International Conference Hall, Kyoto, Japan
Date	October 29 th – November 3 rd , 1979
Organising Committee:	K Fukui and M Kotani
Opening Addresses	K Fukui, P O Löwdin, K Husimi, Y Yukawa
Congress:	There were five associated symposium entitled: <i>New Approaches in Quantum Chemical Methodology</i> (M Kotani, R G Parr (DFT), O Goscinski, F Matsen et al) <i>Structure and Reactivity</i> (M Simonetta, R Bader, R Wyatt) <i>Large Molecules</i> (P O Löwdin, A Veillard, M Basilevsky, K Ohno, E Clementi) <i>Structure and Spectroscopy</i> (J A Pople, T Oka, P W Atkins) <i>Molecular Interactions</i> (J Koutecky, Y T Lee et al, R A Marcus, D P Craig)
Sponsorship:	Financial support was given by: The Science Council of Japan The Japanese Chemical Society
Attendance:	657 participants 133 students 172 foreign participants 43 accompanying persons
Presentations:	362 contributions
Publication:	Papers were published by Wiley in 1980 in the <i>International Journal of Quantum Chemistry</i> 18 , 1-659 (1980). The special editor was J R Sabin. The plenary papers were published as 'Horizons of Quantum Chemistry', eds K Fukui and B Pullman. Reidel (1980)

THE FOURTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

- Place:** University of Uppsala, Uppsala, Sweden
- Date** June 14th – 19th 1982
- Organising Committee:** P-O Löwdin, J-L Calais and O Goscinski
- Congress:** Principal topics of the Congress were:
Quantum Chemical Methods
R Daudel, G Emch, J Linderberg, B Brandow
and J Paldus
Time-Independent Phenomena
E B Wilson, A Davydov, R Berry et al.,
and P v R Schleyer
Time-dependent Phenomena
K Fukui, E Nikitin, R Levine and F Gianturco
Computational Quantum Chemistry
J A Pople R Buenker and S Peyerimhoff
K Morokuma et al., W Kolos and I Shavitt
Surfaces and Catalysis
G Somorjai and J Pendry
Theory of Large Molecules and Solids
J Koutecky, A Overhauser and K Carneiro
Quantum Biology and Quantum Pharmacology
B Pullman, Yu Orchinnikov, P Schuster, R Lavery
and A Pullman
- 2% of the Congress fees were set a-side for the scientific
organisers of Congresses
- Sponsorship:** Financial support was received from:
The Swedish Department of Education
The Nobel Committees in Physics and in Chemistry
The Swedish Natural Science Research Council
Uppsala University
- Attendance:** 450 scientists from 45 nations
300 scientific papers were presented
- Publication:** The plenary lectures were published as “*New Horizons of
Quantum Chemistry*”, *Proceedings of the Fourth International
Congress of Quantum Chemistry*” eds.
P-O Löwdin and B Pullman, Reidel (1983), 468 pages.
Contributed papers were published in the first four issues of the
International Journal of Quantum Chemistry, 1983, **23**, with
1700 pages (eds J-L Calais, O Goscinski).

THE FIFTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

Place:	University of Montreal, Montreal, Canada
Date	August 18 th – 24 th 1985
Organising Committee:	C Sandorfy, W Siebrand and V H Smith
Congress:	<p>Principal topics of the Congress were:</p> <p>Molecular Excited States Systems with Heavy Atoms Light and Particle Scatterings Electron Densities Biomolecular Systems Intermolecular Interactions Molecular Dynamics</p>
Sponsorship:	Financial Support: One-third of the budget and two-thirds of the registration fees was provided by the National Research Council of Canada.
Attendance:	<p>433 participants (245 from North America, 106 from Western Europe, 13 from Eastern Europe, 13 from China, 17 from Third World Countries and 59 students) 46 Invited Speakers (with 15 Chairmen) 345 posters were presented</p>
Publication:	<p>Publication of Proceedings: Papers were published in the <i>International Journal of Quantum Chemistry</i>, 29, pps 177-1685 (1986). Eds J Sabin and M C Zerner).</p> <p>There is an introductory Preface on page v, and a list of participants in pps xi-xl.</p> <p>P-O Löwdin's state-of-the-art lecture is included.</p> <p>The Principal decisions of this year's Academy Meeting was published in the <i>International Journal of Quantum Chemistry</i></p>

THE SIXTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

- Place:** The Hebrew University, Jerusalem, Israel
- Date** August 22nd – 25th 1988
- Organiser:** Joshua Jortner with R D Levine, M Cohen, R Pauncz, M Baer, H Basch, R Gerber, A Goldblum, A Halevi, U Kaldor, A Nitzan, B Scharf, M Shapiro
- Congress:** *The objectives of the Congress were:*
(a) to provide an overview of recent novel developments, advances and directions of research in the broad area of quantum molecular sciences and
(b) to establish strong interaction between the theoretical discipline of quantum molecular sciences and experiments.
A banquet was held at the Knesset
- Topics:*
Molecular Quantum Mechanics
Many-body Theory of Molecular Structure
Intermolecular Forces
Complexes and Clusters
Molecular Spectroscopy
Intramolecular Dynamics
Chemical Reactions
Molecular Dynamics Simulations
Condensed-Phase Chemistry
Surface Phenomena and Catalysis
Quantum Biochemistry
Biophysics
- Sponsorship:** Financial support was received from:
Israeli Universities
Israeli Ministry of Science
Foundation Edmond de Rothschild
Baron Edmond de Rothschild
- Publication:** Proceedings were published in the *International Journal of Quantum Chemistry* **36**, 187-427 (1989), including address by P O Löwdin on 'The Present Status'. Plenary lectures are published by Kluwer 1989 Academic Publishers "Perspectives in Quantum Chemistry" ed. J Jortner and B Pullman

THE SEVENTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

Place:	Palais de l'Europe, Menton, France
Date	July 2 nd – 5 th 1991
Organising Committee:	Lionel Salem (Chairman), Alain Sevin (Executive Secretary) Philippe C Hiberty (Treasurer)
Congress:	The Plenary Lecturers were: G Ertl, W A Goddard, R Hoffmann, W Kohn, W Kutzelnigg, J-P Malrieu, J A Pople, S Shaik, K B Wiberg, and R E Wyatt.
Sponsorship:	An exhibition of computers was organised. Nine private companies were present at the exhibition. Alliant contributed substantially towards financial support.
Attendance:	500 participants 10 Plenary Lecturers 42 Additional Lecturers 313 posters were presented
Satellite Meetings:	<i>Catalysis</i> Organiser: B Bigot <i>Electron Transfer</i> Organiser: M Chanon <i>Recent Methodological Advances in Dynamical and Correlation Calculations</i> Organiser: M Pélissier and X Chapuisat <i>Computer Simulations of Biomolecular Systems</i> Organiser: B Pullman and R Lavery <i>New Materials</i> Organiser: J P Launay and R Portier
Publication:	Papers were not published, but a book of abstracts was edited. The 10 Plenary Lectures were recorded on video.
Acknowledgement:	This information was provided by Philippe Hiberty who wished to record his great pleasure at teaming up with Lionel Salem and Alain Sevin.

THE EIGHTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

Place:	Prague, Czech Republic
Date	June 19 th – 23 rd 1994
Organising Committee:	Rudolf Zahradnik (Chairman), Petr Cársky, Pavel Hobza, Vladimira Bergerova, Jiri Fiser, Zdenek Havlas, Vojtech Hrouda, Pavel Jungwirth, Ivana Paidarova, Rudolf Polak, Vladimir Spirko, Jaroslav Vacek, Jan Vojtik and Jiri Vondrasek
Congress:	<p>The Congress was held in the Municipal Convention Centre (“Palace of Culture”) now Prague Congress Centre). This was the first Congress to be held in a post-communist country. For many researchers from Central and Eastern Europe it was their first opportunity to attend the ICQC. Great efforts were made to make the visit affordable. Charles University provided cheap accommodation in student dormitories but organisers felt they were not very successful in this respect. Reg. fees covered: welcome drink, free pass for all municipal transport and four Congress lunches. The Banquet was 35 USD. Donation of 4000 DM was given to IAQMS.</p>
Attendance:	740 participants; 260 students; 325 acc. persons
Satellite Meetings:	<p><i>Thirty years of density functional theory: concepts and applications</i> June 13th – 16th held in Cracow, Poland Organiser: R Nalewajski</p> <p><i>Molecular modelling in genetics and protein engineering</i> June 15th – 18th held in Sopron, Hungary Organiser: G Naray-Szabo</p> <p><i>Quantum chemical aspects of heterogeneous catalysis</i> June 26th – 28th held in Berlin, Germany Organisers: J Sauer, K Hermann</p> <p><i>Electron correlation in atoms and molecules: new methods and applications</i> June 15th – 18th held in Bratislava, Slovakia Organiser: I Hubac</p>
Publication:	Proceedings published in the <i>Journal of Quantum Chemistry</i> (Per-Olov Löwdin organized the reviewing of papers at the conference (see IJQC 57 265-984 (1996). List of participants pps 985-1016). Book of Abstracts also published.

THE NINTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

Place:	Atlanta, Georgia, USA
Date	June 9 th – June 14 th 1997
Organising Committee:	Keiji Morokuma (Chair); Ernest R Davidson Henry F Schaefer III
Congress:	<p>The Congress took place in the Conference Center, at Emory University. There was a Congress excursion with BBQ lunch at Stone Mountain Park during the afternoon of Thursday June 12th.</p> <p>The Banquet at Emory Conference Center was held in the evening of Saturday, June 14th. All participants were invited to both free of charge.</p>
Sponsorship:	Financial Support: Registration fee + donation from IBM and several other companies and laboratories.
Attendance:	400 plus participants from more than 40 countries 80 invited speakers (four plenary talks in one session and 76 invited talks in two parallel sessions) 380 posters were presented in four evening sessions
Satellite Meetings:	<p><i>Density Functional Theory and Computation</i> June 3rd – 7th at Duke University Organiser: Weitao Yang</p> <p><i>Theoretical Chemistry in Biology</i> June 3rd – 7th at University of Florida Organiser: Mike Zerner</p> <p><i>Structural and Mechanistic Organic Chemistry</i> June 5th – 7th at University of Georgia Organiser: H F Schaefer III</p> <p><i>Quantum Theory of Simulation of Bulk, Surface and Interface Phenomena</i> June 15th – 17th at North Carolina State University Organiser: Mike Whangbo</p> <p><i>Coupled Cluster Theory and Electron Correlation</i> June 15th – 19th at University of Florida Organiser: Rodney Bartlett</p> <p><i>Interplay between Theory and Experiment in Molecular Spectroscopy and Dynamics</i> June 15th – 18th at Memphis, Tennessee Organiser: Peter Pulay</p>
Publication:	There was a Special Issue of the <i>International Journal of Quantum Chemistry</i> 70, 1-239, 241-413 (1998).

THE TENTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

Place:	Palais de l'Europe, Menton, France
Date	June 5 th – June 10 th 2000
Organising Committee:	J-L Rivail (Chairman), S Peyerimhoff, N C Handy and A Pullman
Congress:	<p>There were 41 invited lecturers:</p> <p>E-J Baerends, G Billing, M Blomberg, V Bonacic-Koutecky, D Clary, D Cramer, M Defrancheschi, G Delgado-Barrio, M Dolg, W Domcke, C Froese-Fischer, C Ghio, F Gianturco, B Jeziorski, S Karna, S Kato, W Klopper, I Komaromi, Y Sup Lee, T Lee, U Manthe, C Marian, H-D Meyer, K Mikkelsen, J Olsen, G Pacchioni, F Pauzat, M Robb, C Roothaan, P Rosmus, U Rothlisberger, P Schwerdtfeger, J Snijders, M Sprik, W Thiel, J Tomasi, A van der Avoird, C Van Wüllen, L Visscher, G Voth, H-J Werner</p>
Attendance:	<p>420 participants (complete list in <i>International Journal of Quantum Chemistry</i>, 84, 442-466 (2001) 250 posters were presented in three sessions</p>
Satellite Meetings:	<p>DFT2000 (Menton) Organiser: N C Handy</p>
Publication:	<p>Introduction by J-L Rivail in the <i>International Journal of Quantum Chemistry</i> 84 441 (2001). Papers in the <i>International Journal of Quantum Chemistry</i> 84, 467-758 (2001).</p>

THE ELEVENTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY:

Place:	Bonn (Germany)
Date	July 20 th – 26 th 2003
Scientific Committee:	W Domcke (Muenchen), B Hess (Erlangen), J Manz (Berlin), W Thiel (Muelheim), H-J Werner (Stuttgart)
Organising Committee:	S D Peyerimhoff with C Kronz, J Mekelburger, W Reckien and R Trilling
Congress:	<p>The Congress took place in the historic main building of the Rheinische Friedrich-Wilhelms-Universitaet located in the centre of the city. Originally the residence of the Prince Electors (Kurfuerstliches Residenzschloss); the University was founded in 1818 by the Prussian King Friedrich Wilhelm III. Participants found this location, within walking distance of all sites (the City Hall, Market place, the Rhein, Beethoven's house, hotels, shops and museums) very attractive. Students were still on Campus since it was last week of the summer term. The Welcome Dinner was served in the Arcades of the University. This was followed by the reception given by the Mayor of Bonn in the historic Old City Hall. The Conference Banquet was on a boat cruising up the Rhein from Bonn to Remagen and back on a beautiful summer evening. The Rhein was exceptionally low due to a very dry summer.</p> <p>Guided excursions could be chosen according to scientific or cultural interest:</p> <ul style="list-style-type: none">(1) Arithmeum Musuem (Bonn), with the largest collection in the world of historical mechanical calculating machines plus early electronic computers and some modern VLSI logic chips.(2) Radio-Observatory Effelsberg, successfully operated since 1972 and still one of the two largest full steerable (360 degrees horizontally and 90 degrees vertically) radio telescopes in the world.(3) Bonn on the tracks of Beethoven; a tour to various places closely related to the life of Beethoven.
Sponsorship:	<p>The main sponsor was the Deutsche Forschungsgemeinschaft contributing 30,000 EUR with an additional 10,000 EUR for participants from middle and eastern Europe. The Alexander von Humboldt (AvH) Foundation gave financial support to participants who had AvH Fellowships in previous years and invited these to dinner one evening at the AvH Foundation. The University provided the facilities with support from some staff members. Further support was obtained from the Pinguin</p>

Stiftung (established by a private donation), from Degussa AG and Bayer AG.

Attendance:

535 participants from 48 countries
44 invited speakers gave lectures
378 posters were presented
The opening lecture was held by Ahmed Zewail

Satellite Meetings:

Electron Correlation: Ab initio methods and density Functional theory (July 16 – 19th) at Bad Herrenalb (organizers H-J Werner and J Gauss)
Catalysis (July 16 – 18th) at Muelheim (organizer W Thiel)
Multidimensional Quantum Reaction Dynamics (July 17 – 18th) at Berlin (organizer J. Manz)
Modelling chemical reactivity: from gas-phase to solution and enzymes (July 16 – 18th) at Nancy, France (organizer M Ruiz-Lopez)
100 years Hans Hellmann (1903-1938), Pseudopotentials & Reactions (July 26th) at Bonn (organizer W H E Schwarz)
Relativistic effects in heavy-element chemistry (July 28 – 30th) at Berlin (organizer C van Wüllen)

THE TWELFTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

- Place:** Kyoto Terrsa, Kyoto, Japan
- Date** May 21st – 26th 2006
- Organising Committee:** S Nagakura (Honorary Chair), H Nakatsuji (Chair), K Hirao (Co-Chair) and S Kato (Co-Chair)
- Congress:** There was a half-day conference excursion to the historical sites of Kyoto (Nijo Castle, Heian Shrine, Kiyomizu Temple). The conference banquet was held at the Rihga Royal Hotel Kyoto, with the top solo tsugaru-shamisenist Hiromitsu Agatsuma. There was also a full program for accompanying persons.
- Sponsorship:** Financial Support: Registration fees varied 25,000 - 50,000 yen. Support from the Ministry of Education, Japan, Japanese Society for the Promotion of Science, Epson Foundation, Pharmaceutical Manufacturers of Japan, Commemorative Organisation for Japan World Exposition plus other Japanese Industrial Support.
- Attendance:** 727 participants from 41 countries including 410 persons from Japan
586 Posters: Poster prizes (EURO 500) to P Pyykkö, A I Krylov, H Nakatsuji, R Salomon-Ferrer, C Y Lin.
- Plenary Lecturers:** W Jorgensen, W Kutzelnigg, Y Lee, W M Miller, K Morokuma, S Nagase and R G Parr.
- Invited Lecturers:** E J Baerends, P Cársky, L S Cederbaum, J Cioslowski, D C Clary, W Domcke, M Dupuis, M Ehara, I Frank, L Gagliardi, M S Gordon, S Grimme, A Gross, S Hammes-Schiffer, T U Helgaker, P Hobbs, K N Houk, P Jorgensen, S Kato, K S Kim, K Kitaura, J Komasa, W A Lester, S I Lu, T J Martinez, J Michl, D Mukherjee, T Nakajima, H Nakamura, M Nooijen, J P Perdew, P Piecuch, M A Ratner, H B Schlegel, P R Surjan, Y-D Wu, X Xu, T Yanai, W Yang.
- Satellite Meetings:** *Chemical Accuracy and Beyond* (Tokyo)
Organisers: K Hirao, K Takatsuka and K Yamashita
Electron Dynamics and Spectroscopy (Sendai)
Organisers: Y Fujimura, K Ohno
Large Molecular Systems (Okazaki)
(Organisers: S Nagase)
Reactions in Solution and Biological Systems (Kyoto)
Organiser: S Kato
Material-oriented Quantum Chemistry (Osaka)
Organisers: K Yamaguchi and T Takui

THE THIRTEENTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY:

Place: Helsinki (Finland)

Date June 22-27 (Monday-to-Saturday), 2009

Scientific Committee: J-M André, K Hirao, W H Miller, P Pyykkö, B O Roos

Local Organization Committee: H Häkkinen, L Halonen, M Hotokka, K Laasonen, J Lundell, R M Nieminen, K Nordlund, T Pakkanen, P Pyykkö, T Rantala, D Sundholm, J T Vaara

Congress: The Congress took place on the central campus of the University of Helsinki. The Opening Ceremony and the poster sessions were held in the main building and the other sessions in the Porthania building where a video link coupled the largest lecture hall to another one. The term was already over so these premises were available.

The University was established in Turku in 1640 and moved to Helsinki in 1828. A chair of Chemistry existed since 1761.

A welcome reception at the main building was offered by the University and another reception by the City of Helsinki in the City Hall on Wednesday. The Conference Dinner was held at the Crown Plaza Hotel on Friday.

On Thursday afternoon excursions could be chosen according to general or cultural interests:

(1) Helsinki sight-seeing.

(2) The Nuuksio natural reserve. Within easy bus ride from Helsinki, this area offers unspoiled nature.

(3) Ainola and Hvitträsk. The house of Jean Sibelius and the residence of the three young architects Herman Gesellius, Armas Lindgren and Eliel Saarinen.

Sponsorship: In addition to the hospitality already mentioned, by the University and the City, economic support was obtained from the Federation of Finnish Learned Societies who administers the public support for scientific conferences. The other sponsors included The Association of Finnish Chemical Societies, Svenska Tekniska Vetenskapsakademien i Finland, Finska Kemistsamfundet, Magnus Ehrnrooths Stiftelse, CSC – IT Center for Science and JCTC. PCCP provided the poster prizes. The Helsinki organizers belonged to the Finnish Centre of Excellence for Computational Molecular Science.

Attendance: 671 participants from 54 countries or territories
35 invited speakers gave lectures
489 posters were presented during three sessions

Satellite Meetings:

Molecular Properties: Bridging the Gap between Theory and Experiment, (June 18-21) at Vettre near Oslo, Norway (117 participants).

Materials Oriented Modelling – Catalysis and Interactions in Solid and Condensed Phases (June 28 – July 1 at Stockholm, Sweden (55 participants).

Weather and atmosphere: Excellent.

THE FOURTEENTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY

Place: Boulder, Colorado (USA)

Date June 20 - 25, 2012

Scientific Committee: Josef Michl (Chairman), Mark Gordon, Ken Houk, Keiji Morokuma

Local Organizing Committee: Josef Michl, Joel Eaves, Casev Hynes

Congress: The Congress took place at the University of Colorado. The opening lecture was presented by W. Carl Lineberger. Invited lecturers were Jürgen Gauss, Jean-Luc Brédas, Krishnan Raghavachari, Kim Baldridge, Gustavo Scuseria, Dage Sundholm for Pekka Pyykkö, Garnet A. Mazziotti, Vlasta Bonacic-Koutecky, Edward F. Valeev, Weston Thatcher Borden, Frank E. Harris, Abraham Nitzan, Krzysztof Szalewicz, Eluvathingal D. Jemmis, Takeshi Yanai, Yun-Dong Wu, Shuhua Li, Jin Yong Lee, Ron Shepard, Shigehiko Hayashi, Wim Klopper. Mel Levy

The welcome Reception was at the UMC Terrace. The Conference Banquet at the NCAR Center Green Drive. Excursions took place to the Rocky Mountain National Park

Sponsorship: SILVER SPONSORS: Fujitsu, Hewlett Packard/NVIDIA, Dell, HPC Systems. SUPPORTERS: Hitachi, Ltd., Physical Chemistry Chemical Physics, CT Solution, Chemical Reviews, Wiley

Attendance: 383 participants (107 students, 276 regular) and 26 accompanying persons from 33 countries
28 invited speakers
274 posters were presented in four sessions

Satellite Meetings: *Low-scaling and Unconventional Electronic Structure Techniques* (June 18-22) at Telluride, CO (organizers P. Pulay and G. Scuseria)
Advances in Quantum Chemistry: Interfacing Electronic Structure with Dynamics (June 20-22) at the U. of Minnesota, Minneapolis, MN (organizers M. Gordon and D. Truhlar).
Quantum Chemistry of Heavy Elements (June 20-22) at Santa Fe, NM (organizers R. Martin and E. Batista).

Quantum Mechanics and Molecular Dynamics of Chemical and Biological Reactivity (June 21-23) at UCLA Campus, Los Angeles, CA (organizers K.Houk and A. Alexandrova)
Computational Chemistry at the Petascale (July 1-3) at U.of Illinois, Urbana (organizer Th.Dunning),
Coupled-Cluster Theory and Related Techniques (July 1-3) at Boulder, CO (organizers J.Stanton and J. Gauss)

THE FIFTEENTH INTERNATIONAL CONGRESS OF QUANTUM CHEMISTRY:

- Place:** Beijing (China)
- Date** June 8th – 13th 2015
- Organizing Committee:** Zhigang Shuai, Weihai Fang, Wenjian Liu, and Weitao Yang
- Scientific Committee:** served by the Theoretical Chemistry Committee of the Chinese Chemical Society (CCS)
- Congress:** The Congress took place in the New Tsinghua Amphitheatre within the beautiful campus of Tsinghua University, which was built in the occasion of the centennial celebration for the establishment of the University in 2011. Thus, the theatre has 2011 comfortable seats. The campus was rated as one of the fourteen most beautiful university campuses in the world by FORBES magazine in the May issue of 2010, the only one chosen from Asia. The IAQMS banquet was served in Tingli Restaurant inside the Summer Palace. The Congress Welcome Dinner was served in the basement of the theatre. The Conference Banquet took place in the Liaoning Mansion hotel nearby the University campus. And all the meals are covered by registration and are served in the GuanChouYuan university cafeteria. Invited speakers and IAQMS members are welcomed by volunteers and picked up in the airport upon arrival.
- Guided excursion was organized for a trip to the Great Wall of China in Dadaling in the afternoon of June 11th.
- Sponsorship:** The Chinese Chemical Society and the Department of Chemistry of Tsinghua University have provided a team of 15 staff members during the Congress as well as most of the organizing efforts more than one year prior to the Congress. The Tsinghua University provided all the venues including ~ 70 on-campus hotel rooms at a well discounted rate.
- Other sponsors are from industry: 50,000 YUAN from HPC systems; 20,000 YUAN from AIP-The Journal of Chemical Physics; 20,000 YUAN Paratera (Beijing); 20,000 YUAN from Yuehaiyangbo Technology Co. (Beijing); 15,000 YUAN from Springer (Shanghai); 15,000 YUAN from Wuzhou Tech. (Guangzhou); 10,000 YUAN from Tech-Box Tech Co. (Beijing). (1EURO = 7 YUAN at the time)
- The Congress provided exhibition tables free of charge for International Journal of Quantum Chemistry special issue "Theoretical Chemistry in China" (Elsevier) and Science China Chemistry for one theoretical chemistry special issue.
- Attendance:** 1000 participants from 43 countries/areas.

39 invited speakers including two Nobel Laureates Rudolph Marcus and Roald Hoffmann presented lectures.
600 posters were presented

Satellite Meetings:

The Frontiers of Computational Catalysis (May 31st – June 2nd)
at Beijing (organizer: Jun Li)
Recent Advances in Electronic Structure Theory (June 1st – 6th)
at Nanjing (organizer: Shuhua Li)
Theoretical Challenges in Small Molecule Dynamics
(July 2nd – 6th) at Dalian (organizers: Donghui Zhang, Keli Han,
Millard Alexander)
Recent Advances in Quantum Dynamics and Thermodynamics
(June 4th – 7th) at Beijing (organizers: Jian Liu, Yiqin Gao)
*Modeling and Simulation of biological and Macromolecular
systems* (June 4th – 6th) at Changchun (organizers: Jiali Gao,
Hongxing Zhang)
The Chemical Bonds at the 21st Century (June 14th – 18th) at
Xiamen (organizer: Wei Wu)
Advances in Modeling of Nano Materials (June 14th – 17th) at
Hefei (Organizers: Jinlong Yang, Yi Luo)
New Frontiers of Relativistic Quantum Chemistry (June 13th –
16th) at Beijing (Organizer: Wenjian Liu)
*Novel Computational Methods for Quantitative Electronic
Structure Calculations* (June 16th – 20th) at Kobe, Japan
(Organizers: Seiichiro Ten-no, Kimihiko Hirao)

4 COMMENTARIES

In the early 1980's I had heard of IAQMS, and towards the end of that decade it was a challenge to become a member. I was therefore truly delighted to become a member in 1988, primarily because this was a form of international recognition for my work in quantum chemistry. My teachers (Boys, Parr, Miller, Schaefer) were all members, and this gave additional pleasure.

The first impression of my first Academy meeting was the absolute amazement that I had ever managed to be elected. The election procedures are truly outstanding: the careful discussion of all the candidates (from those present with input from absentees), the very rigorous voting procedures which seem designed to prevent any clique pushing through a favoured candidate. Above all, members are elected solely on their academic distinction in the field of quantum molecular science. In this way the elections give members from many countries: it is one of the attractions of our subject that, thanks especially to computational advances, it is possible to undertake research in our subject in all parts of the world. It is particularly pleasing that once elected, you are a member for life; this allows the more senior of us to watch the upcoming developments of the field.

I was taught as an undergraduate that it was important to know the names of the key players in the field. When I was elected all Founding members attended the meetings (Daudel, Pullman, Pople, Löwdin, Löwdin, Parr), and it was an honour to listen to these distinguished scientists. It was a highlight to see Fischer-Hjalmers at a meeting (and of course many others, but I knew of her work with my PhD examiner, Coulson).

Upon my appointment as Secretary, it was decided to create a booklet of academy members, one page per member. My excellent secretary (Mrs Sue Harding) then contacted all members, requesting a photograph, a potted cv and a description of their science. In this way we knew many members: some replied quickly (especially the senior members), some were very slow, some scientific inputs were exceedingly brief whilst others gave much detail. This was an extremely enjoyable exercise!

One of the important aspects of academy meetings is to discuss forthcoming International Congresses (held every three years). We discuss the venue (it is important to be International). But most important, we select the Invited Speakers, enabling upcoming younger scientists known to some members, to be invited. These Congresses are not dominated by Academy members; instead they should reflect the direction of our science. The Invited Speaker list then attracts a very good attendance, and in this way promotes the field. I view the Congresses to be the most important Academy activity.

I cannot close before acknowledging the generosity of the city of Menton through its authorities. They host us at each Academy meeting, they provide the venue (The Villa Maria Serena), and if we hold a Congress in Menton, they are very generous to us with all their help. I wish it was customary for cities in my country to sponsor particular academic activities. Thank you Menton!

Nicholas Handy