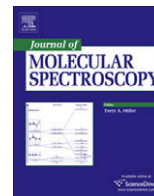




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## PRAHA2008. The 20th International Conference on High Resolution Molecular Spectroscopy Prague, Czech Republic, September 2–6, 2008

### 1. Introduction

The present special issue of Journal of Molecular Spectroscopy has a dual purpose. Primarily, it collects papers resulting from work presented at the 20th International Conference on High Resolution Molecular Spectroscopy (PRAHA2008), which took place from September 2 to September 6, 2008, in Prague-Dejvice, Czech Republic, and in this context it briefly reports the proceedings at PRAHA2008 (Section 2). However, as PRAHA2008 was the 20th “Prague meeting”, the history of the conference series is also outlined (Section 3).

### 2. The PRAHA2008 conference

The local organization of PRAHA2008 was jointly undertaken by the Institute of Chemical Technology in Prague, the Academy of Sciences of the Czech Republic (represented by the J. Heyrovský Institute of Physical Chemistry and the Institute of Organic Chemistry and Biochemistry), the Czech Technical University (whose buildings served as conference venue), and the Ioannes Marcus Marci Spectroscopic Society.

The conference had 235 participants from 28 countries. There were 212 scientific presentations of which 12 were 45-minute invited talks, 34 were 15-minute contributed talks, and 166 were posters.

The presentations at the conference were concerned with observation, measurement, and analysis of high resolution rotational, vibrational, or electronic spectra of molecules, with theory assisting the prediction, simulation, and interpretation of such molecular spectra, and with the applications of high-resolution molecular spectroscopy techniques in related fields such as atmospheric research, astrophysics, astrochemistry, and biological studies. This is reflected by the papers in the present special issue and by the 12 invited lectures which were the main events of the conference. Here, new developments and extensions of experimental spectroscopic techniques were described by **Kodo Kawase** (*Nagoya University, Japan*) who spoke about THz-wave generation and its applications in imaging techniques. **Zbigniew Kisiel** (*Polish Academy of Sciences, Warsaw, Poland*) gave new examples of the analysis of broadband rotational spectra, and **Juan Carlos López** (*Universidad de Valladolid, Spain*) showed how, by means of jet-cooled rotational spectroscopy of laser-ablated biomolecules, the gas phase structures of neutral amino acids can be determined. **Hans Jürgen Neusser** (*Technische Universität München, Munich, Germany*) dis-

cussed, at the other end of the electromagnetic spectrum, how high-resolution UV spectroscopy can be used to study weak interactions and conformational structures for flexible molecules and clusters.

The interplay between high-resolution molecular spectroscopy and *ab initio* theory was discussed by **Walter Thiel** (*Max-Planck-Institut für Kohlenforschung, Mülheim/Ruhr, Germany*). **Yunjie Xu** (*University of Alberta, Edmonton, Alta., Canada*) also employed *ab initio* methods, in conjunction with high-resolution spectroscopy, in order to explore chirality and chiral recognition at the molecular level.

Applications in atmospheric studies were presented by **Valery Perevalov** (*Institute of Atmospheric Optics, Russian Academy of Sciences, Tomsk, Russia*) in a talk about global modelling of high-resolution spectra of linear molecules and the inclusion of the results in spectroscopic databases. **Sandra Brünken** (*Harvard Smithsonian Center for Astrophysics, Cambridge, MA, U.S.A.*) reported new observations of molecular anions in the laboratory and in space. Other astrophysical applications were discussed by **Robert Georges** (*Université de Rennes I, France*) in a talk on infrared spectroscopy of gases at high temperatures. It was initially planned that **Stephan Schlemmer** (*Universität zu Köln, Cologne, Germany*) would talk about the spectroscopy of stored cold ions. Unfortunately, Prof. Schlemmer fell ill and could not come to Prague, and his talk was given by **Thomas F. Giesen** (*Universität zu Köln, Cologne, Germany*).

In the afternoon of Wednesday, September 3, 2008, the ceremonial Ioannes Marcus Marci Session (held under the auspices of the Lord Mayor of Prague) took place in the Prague City Hall Auditorium, a historic lecture hall in central Prague. The featured Ioannes Marcus Marci speakers were **Terry A. Miller** (*The Ohio State University, Columbus, OH, U.S.A.*) and **Thomas L. Wilson** (*European Southern Observatory, Garching near Munich, Germany*). Prof. Miller spoke on the use of spectroscopy to probe reaction intermediates in combustion studies and atmospheric chemistry, while Prof. Wilson described the current status and scientific potential of the Atacama large mm/sub-mm array. The session concluded with Profs. Miller, Wilson, and Prof. **Per Jensen** (*Bergische Universität Wuppertal, Germany*) being awarded the Ioannes Marcus Marci Medal of the Ioannes Marcus Marci Spectroscopic Society. In the evening after the session, the participants were invited to a reception in the state apartment of the Lord Mayor of Prague.

The tradition of the Liblice/PRAHA conferences was continued in that a chamber concert was organized for the participants in

the evening of Friday, September 5, 2008, in the Magna Aula of the Carolinum (the Gothic-style historical Grand Auditorium of Charles University). The *Bennewitz Quartet* played polkas by Bedřich Smetana and the “Quintet in C Major for Two Violoncellos” by Franz Schubert. Before the concert, three Josef Plíva Prizes were awarded for the best student contributions. These prizes were won by

- **Oliver Baum**, *I. Physikalisches Institut, Universität zu Köln, Cologne, Germany*, for a poster entitled “Internal Rotation Tunneling in Four-Atomic Skew-Chain Molecules.”
- **Tarekegn Chimdi**, *Department of Chemistry, Monash University, Clayton, Vic., Australia*, for a poster entitled “Ro-vibrational Analysis of the  $\nu_9$  and  $\nu_{16}$  Bands of R152A.”
- **Lucie Kolesníková**, *Faculty of Chemical Engineering, Institute of Chemical Technology, Prague, Czech Republic*, for a poster entitled “Fine (and hyperfine) Structures in Rotational Spectra of the FSO<sub>3</sub>-Radical.”

The winners were selected by a panel of anonymous judges. The prizes consisted of a diploma, and the recipients were given a selection of books.

We think that PRAHA2008 was a successful conference with a high scientific standard and a good time being had by all. In 2010, the 21st conference in the series will take place in Poznań, Poland, September 7–11, with **Marek Kręglewski** as principal organizer.

### 3. A brief history of the Prague spectroscopy conference

To mark the occasion of the 20th International Conference on High Resolution Molecular Spectroscopy, one of us (JTH) gave, at the Ioannes Marcus Marci Session, an account of some of the early conferences in the series. We use his presentation as the starting point for an outline of the history of the “International Conference” (or “Prague meeting”) series.

The genesis of the “Prague meeting” and the “Dijon meeting” (i.e., the “International Colloquia on High Resolution Molecular Spectroscopy” held in Western Europe in odd years, every second time in Dijon, France) was at a very small conference at NRC Ottawa in July 1968 attended by JTH and (among others) **Josef Plíva** (Czechoslovakia), **Gilbert Amat** (France), and **Ian M. Mills** (United Kingdom). Their idea was to have a high-resolution molecular spectroscopy meeting, alternately in Eastern and Western Europe, both modeled on the US Columbus meeting (the annual “Ohio State Symposium on Molecular Spectroscopy”), i.e., with a central focus on many presentations by graduate students and post-doctoral fellows. Plíva, Amat, and Mills believed there was a need for meetings in Europe that were not restricted by invitation or by cost to established, senior scientists.

The invasion of Czechoslovakia by Warsaw pact forces in August 1968 presumably influenced the planning of the Prague meetings, but in September 1970 the first meeting in the series was held in Prague (at the Czech Technical University) with **Dušan Papoušek** (of the J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences) as principal organizer. Dr. Papoušek remained the principal organizer of the meetings up to and including the 11th meeting in Dobříš in 1990. The 2nd meeting took place in Prague in 1972, and the third (1974) to tenth (1988) meetings all were held at the legendary Liblice Castle, a small chateau in the country north of Prague, belonging to the Czechoslovak Academy of Sciences. In the 1970's and 80's, the Iron Curtain was firmly in place, but Prague was still relatively easily accessible both from East and West, and the Liblice meeting became a unique meeting place for Eastern and Western scientists. Many East–West scientific collabora-

tions developed and many visits were arranged. Also, even though the Czechoslovak security forces certainly were eyeing visitors from the West with great distrust, Liblice seemed to be remarkably “surveillance free”. The atmosphere of the Liblice meetings was—in the words of JTH—“informal and playful, like a high-school party that your parents didn't want you to attend”. There were about 120 participants, since this was the number that could be seated in the lecture hall. Everybody ate in Liblice castle, and most of the participants slept there, mostly in dormitory-type rooms with several beds. Participants requiring rooms to themselves stayed in a hotel in the nearby town of Mělník (where the autumnal sugar-beet-processing campaigns in the neighbouring sugar factory tended to consume all available hot water, making for cold showers for the participants), and those requiring very cheap accommodation camped in nearby campgrounds. There were evening gatherings in the castle dining room, a Tuesday-night picnic with barbecued sausages, a Thursday-night chamber concert (with the highly talented **Talich Quartet**), and occasional mushroom-hunting in the surrounding forests (with subsequent mushroom-eating in the castle). So it was easy to get to know everybody. For the erstwhile participants, the eight Liblice conferences spanning 16 years are an inexhaustible source of nostalgia.

After the political change in Czechoslovakia towards the end of 1989, Prague became very easily accessible to citizens of Western countries, for whom the visa duty generally was abolished during the first half of 1990. Consequently, the number of prospective participants for the 11th meeting in 1990 greatly exceeded the 120 that could be accommodated in Liblice, and it became necessary to move the meeting to the privately-owned castle in Dobříš south of Prague (This happened at rather short notice and so the 1990 PROGRAM OF SESSIONS/ABSTRACTS OF PAPERS booklet has “Liblice near” pasted over with a strip of paper on the outside cover). At the 11th meeting, the running of the conference series was “modernized”; it was made similar to that of the “Dijon meetings” and an international steering committee was instituted with **Jon T. Hougen** as the first chairman and **Michel Betrencourt**, **Gianfranco DiLorenzo**, **Vladimir Tyuterev**, and **Manfred Winnewisser** as members. The 12th meeting also took place at Dobříš castle with **Vladimír Špirko** as chairman of the local organizing committee. Vladimír Špirko remained chairman of the local organizing committee up to and including the 2000 conference; at all subsequent conferences **Štěpán Urban** (who was executive chairman in 2000) has had this position.

In 1994, the Prague team had organized 12 successive conferences and were happy to let the meeting make an excursion outside Czechoslovakia: The 13th meeting was held in Poznań, Poland, with **Jerzy Konarski** as principal organizer. New members were elected for the international steering committee and **Per Jensen** replaced Jon T. Hougen as chairman. Per Jensen remained chairman until 2006, when he was replaced by **Koichi M.T. Yamada**.

The 14th meeting returned to Prague and took place in buildings of Charles University in Prague-Troja in September 1996. At that time, the principle of branding had been discovered and the new brand name **PRAHA96** was introduced.

The 15th and 16th meetings, PRAHA98 and PRAHA2000 (as it did not appear quite appropriate to call the 2000 meeting PRAHA00) also took place in the building complex in Prague-Troja. Less than three weeks before PRAHA2002, however, the probably most dramatic incident in the conference history occurred. There was severe flooding in Prague 19 days before the conference beginning, and the conference venue in Prague-Troja was basically made uninhabitable. In a heroic effort of the local organizing committee, the conference was relocated in minimum time to buildings of the Institute of Chemical Technology and the Czech Technical Univer-

sity in Prague-Dejvice, and it ran extremely well in spite of all the difficulties. The conference location in Prague-Dejvice was seen to have many advantages relative to that in Prague-Troja (in particular a much better lecture hall and better dormitory rooms), and the PRAHA2004, PRAHA2006, and PRAHA2008 meetings have all been held in Prague-Dejvice.

A fairly recent addition to the conference is the Ioannes Marcus Marci (IMM) Session held under the auspices of the Ioannes Marcus Marci Spectroscopic Society (a.k.a. the Czech Spectroscopic Society) and of the Lord Mayor of Prague. The first of these sessions took place at PRAHA2000 with the Nobel Laureate **Harold W. Kroto** as IMM speaker. The IMM speakers include the Nobel Laureates **Ahmed Zewail** (2002) and **Theodor W. Hänsch** (2006) together with other distinguished scientists: **Gisbert Winnewisser** (2000), **Jon T. Hougen** (2002), **Richard J. Saykally** (2004), **Ian M. Mills** (2004), **William Klemperer** (2004), **Philip R. Bunker** (2006) and, as mentioned above, **Terry A. Miller** (2008) and **Thomas L. Wilson** (2008).

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