

*B. P. Winnemurser*

**III<sup>rd</sup> INTERNATIONAL SEMINAR  
ON HIGH RESOLUTION  
INFRARED SPECTROSCOPY**

**LIBLICE NEAR PRAGUE**

**SEPTEMBER 2 - 6, 1974**

## C o n t e n t s

|                             |           |           |
|-----------------------------|-----------|-----------|
| <b>Program of Sessions</b>  | . . . . . | <b>1</b>  |
| <b>Social Program</b>       | . . . . . | <b>10</b> |
| <b>Abstracts of Papers</b>  | . . . . . | <b>11</b> |
| <b>List of Participants</b> | . . . . . | <b>44</b> |

IIIrd INTERNATIONAL SEMINAR ON HIGH RESOLUTION  
INFRARED SPECTROSCOPY, LIBLICE NEAR PRAGUE,  
SEPTEMBER 2 - 6, 1974

---

Program of Sessions

Monday, September 2

Opening Ceremony 9.00 a.m.

Morning Session: (Chairman - Prof. I. Kovács)

Opening Talks

- A1. W. Gordy (Department of Physics, Duke University,  
Durham, Carolina, U.S.A):  
"Far Infrared Spectroscopy with Microwave  
Techniques" (invited paper) 9.30 - 10.20 a.m.
- A2. O.A. Tumanov (Institute for Spectroscopy, Academy of  
Sciences, USSR):  
"Methods of Nonlinear Laser Spectroscopy  
Without Doppler Broadening" (invited paper)  
10.30 - 11.00 a.m.
- A3. Yu.S. Makushkin and V.I.G. Tyuterev (Institute of  
Atmospheric Optics, Siberian Branch of the  
Soviet Academy of Sciences, Tomsk, USSR):  
"The Treatment of Centrifugal Distortion  
Effects for the Molecules with a Tetragonal  
Symmetry by the Contact Transformations"  
(invited paper) 11.05 - 11.30 a.m.

not here

Henni - B1

- A4. V.M. Blinov, V.N. Bryukhanov, V.Ts. Gomboev,  
Yu.S. Makushkin, V.I. Perevalov and Vl.G. Tyuterev  
(Institute of Atmospheric Optics, Siberian  
Branch of the Soviet Academy of Sciences,  
Tomsk, USSR):

"Effective Rotational Constants and Centrifugal  
Distortion Constants of Polyatomic Molecules"

11.35 - 11.55 a.m.

*Parker*

Afternoon Session (Chairman Dr. J.T. ~~Hogen~~)

Techniques of High Resolution Infrared, Submillimeter and  
Laser Spectroscopy

- B1. L. Henry (Laboratoire de Spectromie Moleculaire,  
Université de Paris VI, France):

"Advances in High Resolution Infrared  
Spectroscopy" (invited paper)

2.00 - 2.50 p.m.

- B2. A.F. Krupnov (Radiophysical Research Institute, Gorky,  
USSR):

"Broad Band Gas Microwave Spectroscopy in  
Submillimeter Wave Range: Methods and  
Investigations" (invited paper)

3.00 - 3.50 p.m.

- Zhishin*  
*p. 45*  
B3. H. Jones (Universität Ulm, Abteilung der Physikalischen  
Chemie, BRD):

"Infrared-Microwave Double Resonance With a  
Spin-Flip Raman Laser"

4.00 - 4.30 p.m.

- B4. H.A. Dijkerman (University of Utrecht, Holland):

"Lamb-Dip Spectroscopy in the Microwave  
Region With an Open Cavity"

4.35 - 5.00 p.m.

- B5. ~~R.C. Milward~~ (Polytec GmbH and Co, Reichenbach-Karlsruhe,  
BRD):

"Recent Advances in Commercial Spectrometers  
for the Submillimeter Wavelength Region"

5.05 - 5.30 p.m.

*Schuy*

Tuesday, September 3

Morning Session: (Chairman - Dr. J. Bordé)

Basic Theory, Molecules in External Fields, Force Constant Calculations

- C1. M.R. Aliev (Institute for Spectroscopy, Academy of Sciences, USSR):  
"Classical Approach, Contact Transformations, and Hypervirial Theorems in the Theory of Molecular Vibration-Rotation Spectra"  
(invited paper) 9.00 - 9.30 a.m.
- C2. J.K.G. Watson (Department of Physics, The Ohio State University, U.S.A.):  
"Molecular Symmetry in Electric and Magnetic Fields"  
9.35 - 10.00 a.m.
- C3. J.T. Hougen<sup>1</sup>, H.E. Radford<sup>2</sup>, K.M. Evenson<sup>3</sup>, and C.J. Howard<sup>4</sup>  
(1 National Bureau of Standards, Molecular Spectroscopy Section, Washington DC 20234, U.S.A.  
2 Smithsonian Astrophysical Observatory, Cambridge MA 02138, U.S.A.  
3 National Bureau of Standards, Boulder CO 80302, U.S.A.  
4 National Oceanic and Atmospheric Administration, Boulder CO 80302, U.S.A.)  
"The Laser Zeeman Rotational Spectrum of HO<sub>2</sub>"  
(invited paper) 10.15 - 10.40 a.m.
- C4. I. Kovács, P. Facher (Department of Atomic Physics, Polytechnical University, Budapest, Hungary):  
"Fine Structure of the  ${}^7\Sigma$  and  ${}^7\Pi$  States in Diatomic Molecules" (invited paper)  
10.45 - 11.15 a.m.
- C5. K.H. Schmidt and A. Müller (Lehrstuhl für Anorganische Chemie der Universität Dortmund, BRD):  
"Vibrational Spectra and Force Constants of Transition Metal Complexes Using Metal Isotopes,  ${}^{14}\text{N}/{}^{15}\text{N}$ , and H/D Shifts"  
11.25 - 11.40 a.m.

- C6. V. Špirko<sup>1</sup> and G.K. Speirs<sup>2</sup> (1 Department of Molecular Spectroscopy, The J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague, 2 University of Aberdeen, Scotland):

"Application of Monte Carlo Method to Anharmonic Force Constants Calculations"

11.45 - 12.10 a.m.

Afternoon Session: (Chairman - Dr. J.M.R. Stone)

Techniques of High Resolution Infrared Spectroscopy

- D1. V.S. Bukreev<sup>1</sup>, A.A. Balashov<sup>1</sup> and G.N. Zhizhin<sup>2</sup>  
(1 Central Construction Bureau of Unique Scientific Instruments, Academy of Sciences, USSR, 2 Institute of Spectroscopy, Academy of Sciences, USSR):

"A High Resolution Fourier Transform Spectrometer"

2.00 - 2.30 p.m.

- D2. R. Sovička, M. Holub, M. Matucha (Department of Molecular Spectroscopy, The J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague):

"Description of the McCubbin Optical Arrangement of the High Resolution Grating Infrared Spectrometer"

2.40 - 3.00 p.m.

- D3. A. Röseler (Zentralinstitut für Optik und Spektroskopie, Akademie der Wissenschaften, Berlin, DDR):

"Beugungsbedingte Apparatfunktion von Doppelmonochromatoren"

3.05 - 3.25 p.m.

Theory of Vibration-Rotation Molecular Spectra

- D4. J. Bordé (Laboratoire de Physique Moléculaire et d'Optique Atmosphérique, C.N.R.S., Orsay, France):

"Calculated Vibration-Rotation Interaction in the Line Intensities of  $^{12}\text{C}^{16}\text{O}_2$ "

3.40 - 4.00 p.m.

- D5. J.M. Flaud and C. Camy-Peyret (Laboratoire de Physique Moléculaire et d'Optique Atmosphérique, C.N.R.S., Orsay, France):  
"Method of Calculation of the Vibration-Rotation Energy Levels and Intensities for H<sub>2</sub>O Type Molecules. Application to the  $2\nu_2$ ,  $\nu_1$  and  $\nu_3$  Band of H<sub>2</sub><sup>16</sup>O" 4.05 - 4.25 p.m.
- D6. L. Nemes (Central Research Institute for Chemistry, Hungarian Academy of Sciences, Budapest, Hungary):  
"Jacobian Elements for Multiple Coriolis Perturbations" 4.35 - 4.55 p.m.
- D7. Yu.S. Makushkin and O.N. Ulenikov (Institute of Atmospheric Optics, Siberian Branch of the Soviet Academy of Sciences, Tomsk, USSR):  
"The Effect of Deviation from Born-Oppenheimer Approximation on Molecular and Spectroscopic Parameters" 5.00 - 5.20 p.m.
- D8. O.K. Voytsekhovskaya and Yu.S. Makushkin (Institute of Atmospheric Optics, Siberian Branch of the Soviet Academy of Sciences, Tomsk, USSR):  
"An Analysis of Vibration-Rotation Interactions Effect on Line Intensities of the Asymmetric Top Type Molecules" 5.25 - 5.45 p.m.
- D9. R. Tipping (Physics Department, Memorial University St. Johns, New Foundland, Canada):  
"Classical Treatment of Vibration-Rotation Intensities for the Morse Oscillator" 6.00 - 6.20 p.m.
- D10. J.M.R. Stone (Université de Sherbrooke, Québec, Canada):  
"The Large Amplitude Motion-Rotation Hamiltonian for Four Atomic Molecules: Application to HCNO and HNCO"  
(last minute paper, will be scheduled later on)

+ A3  
+ A4

M. Kumanova: CNDO study, internal rotation

CO<sub>2</sub> CO<sub>12</sub> CO<sub>13</sub>

Wednesday, September 4

Morning Session: (Chairman - Prof. P.M. ~~Barker~~)

Molecules With Large Amplitude Motions

- Hougel*
- E1. M. and B. Winnewisser (Physikalisch-Chemisches Institut, Justus Liebig-Universität, Giessen, BRD):  
"Why it Took 174 Years to Understand the Structure of Fulminic Acid" (invited paper)  
9.00 - 9.30 a.m.
- E2. P.M. Parker (Department of Physics, Michigan State University, USA):  
"Isotopic Substitution in Nonlinear Triatomic Molecules"  
9.40 - 10.00 a.m.
- E3. V. Špirko<sup>1</sup>, J.M.R. Stone<sup>2</sup>, and D. Papoušek<sup>1</sup> (1 Department of Molecular Spectroscopy, The J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague, 2 The University of Sherbrooke, Canada):  
"Centrifugal Distortion, Coriolis Interactions, and Force Field in  $^{14}\text{NH}_3$ ,  $^{15}\text{NH}_3$ ,  $^{14}\text{ND}_3$  and  $^{14}\text{NT}_3$ "  
10.15 - 10.35 a.m.
- E4. V. Danielis, D. Papoušek, V. Špirko and M. Horák (Department of Molecular Spectroscopy, The J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague):  
"Vibration-Inversion-Rotation Hamiltonian for  $\text{NH}_2\text{D}$  and  $\text{ND}_2\text{H}$ "  
10.40 - 11.00 a.m.
- E5. J. Sheridan (School of Physical and Molecular Sciences, University College of North Wales, Bangor, England):  
"Microwave Spectra With Large Vibrational Contributions From Proton Tunnelling"  
11.05 - 11.25 a.m.
- E6. L.L. Boyle and J.H. Bennett (University Chemical Laboratory, Canterbury, England):  
"Highlights in the Theory of Non-Rigid Molecules"  
11.30 - 12.10 a.m.

D70 ~~Am~~ Stone



- E7. V. Špirko (Department of Molecular Spectroscopy, The J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague):

"A Possible Extension of the Numerov Method to Multidimensional Schrödinger Equations"

12.15 - 12.30 a.m.

Afternoon Session: (Chairman - Dr. D. Van Lerberghe)

Analysis of High-Resolution Infrared Spectra

- F1. G. Steenbeckeliers<sup>1</sup>, D. Van Lerberghe<sup>2</sup>, R. Van Riet<sup>1</sup>, and J. Bellet<sup>3</sup> (1 Université Catholique de Louvain, Louvain-La-Neuve, Belgique, 2 Institut de Physique Corpusculaire, Louvain-La-Neuve, Belgique, 3 Université Lille-I, France):  
"Microwave, Infrared and Laser Spectrum of SO<sub>2</sub>"  
2.00 - 2.45 p.m.
- F2. A.G. Maki (Optical Physics Division, National Bureau of Standards, Washington, U.S.A.):  
"High Resolution Infrared Measurements on Ozone (O<sub>3</sub>), Allene (C<sub>3</sub>H<sub>4</sub>), and Hydrogen Cyanide"  
2.50 - 3.20 p.m.
- F3. M. Betrencourt and M. Morillon-Chapey (Laboratoire d'Infrarouge, Campus d'Orsay, France):  
"High Resolution Spectrum of CH<sub>3</sub>Br in the Range of 2970 cm<sup>-1</sup>"  
3.30 - 3.50 p.m.
- F4. C. Betrencourt (Laboratoire d'Infrarouge, Campus d'Orsay, France):  
"Contribution a l'Etude de la Composante Parallele de la Bande  $\nu_2 + 2\nu_5$  vers 4160 cm<sup>-1</sup>"  
3.55 - 4.20 p.m.
- ~~F5.~~ C. Alamichel<sup>1</sup>, G. Graner<sup>1</sup>, H. Bürger<sup>2</sup>, S. Biedermann<sup>2</sup> and A. Ruoff<sup>3</sup> (1 Laboratoire d'Infrarouge, Campus d'Orsay, France, 2 Institut für anorganische Chemie der TH Braunschweig, BRD, 3 Sektion für Schwingungsspektroskopie, Universität Ulm, BRD):  
"A New Investigation of the  $\nu_1$  and  $2\nu_5$  Bands of CF<sub>3</sub><sup>35</sup>Cl and CF<sub>3</sub><sup>37</sup>Cl"  
4.25 - 4.45 p.m.

F6. J. Mink and F. Kling (Institute of Isotopes of the Hungarian Academy of Sciences, Budapest, Hungary):

"Medium Resolution Vibration-Rotation Spectra and Molecular Force Field of

$^{14}\text{C}_2\text{H}_2$  and  $^{14}\text{C}_6\text{H}_6$  Molecules"

5.00 - 5.20 p.m.

F7. J. Mink<sup>1</sup>, P.L. Goggin<sup>2</sup> and G. Kemény<sup>1</sup> (1 Institute of Isotopes of the Hungarian Academy of Sciences, Budapest, Hungary, 2 Inorganic Chemistry Department, University of Bristol, Bristol, England):

"Far Infrared and Raman Spectra, and Lattice Vibrations of Methyl Mercury Halides"

5.30 - 5.50 p.m.

Thursday, September 5

Morning: Sight-seeing Tour

Afternoon: Excursion to the Infrared Laboratory of the J. Heyrovský Institute of Physical Chemistry and Electrochemistry in Prague

Friday, September 6

Morning Session: (Chairman - Dr. A.G. Maki)

High Resolution Raman and Infrared Spectroscopy

G1. S. Brodersen and F. Rasmussen (Department of Chemistry, Aarhus University, Denmark):

"Recent Results in High Resolution Raman Spectroscopy"

9.00 - 9.30 a.m.

G2. K. Altman and G. Strey (Sektion der Physik, Universität München, BRD):

"Rotational Structure of Hyper-Raman-Bands"

9.40 - 10.10 a.m.

G3. A. Fayt (Institut de Physique Corpusculaire Chemin du Cyclotron, Louvain-La-Neuve, Belgium):

"High Resolution Spectrum of HD<sup>18</sup>O"

10.25 - 10.55 a.m.

revised



- G4. P. Pinson and J.C. Deroche (Laboratoire d'Infrarouge, Orsay, France):  
"High Resolution Spectrum of  $\text{CH}_2\text{D}_2$  near  $8\mu$ "  
11.00 - 11.30 a.m.
- G5. F. König and A. Müller (Lehrstuhl für Anorganische Chemie der Universität Dortmund, BRD):  
"Gas Phase Spectra and Matrix Isolation Spectra of Some Tetrachlorides With Pure Metal and Chlorine Isotopes"  
11.40 - 12.00 a.m.
- G6. Š. Urban and M. Horák (Department of Molecular Spectroscopy, The J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague):  
"A New Function Describing Infrared Band Profiles"  
12.05 - 12.20 a.m.

The Meeting will end on Friday, September 6th, at lunch time. Transports from Liblice will start after lunch and the last transport from Liblice to Prague will be provided in the afternoon from the Castle at 4.00 p.m. Should your travel plans require a hotel reservation in Prague after the Meeting or if you wish to be accomodated in Prague during the Seminar, please, contact our Travel Agency ČEDOK. Unfortunately, it is impossible for the Institute to secure any accomodation.

Organizing Committee:

D.Papoušek (Chairman), V.Špirko (Deputy Chairman),  
R.Sovička, M.Horák, V.Zedlerová (Secretary), J.Pitrová  
(Social Program), M.Holub (Technician), A.Kožišková,  
L.Bureš (Economical).

Address: The J. Heyrovský Institute of Physical Chemistry  
and Electrochemistry, Czechoslovak Academy of  
Sciences, Flemingovo nám.2, 160 00 PRAGUE 6,  
Czechoslovakia

Social Program

Monday Evening:

Cocktail Party

8 1/2 p.m.

*After supper*

Tuesday Evening:

Chamber Music

7:30

(B.Smetana and A.Dvořák)

8.00 p.m.

Wednesday Evening:

~~Banquet~~

*Barbecue!*

7.00 p.m.

Thursday Morning:

Sight-Seeing Tour

Starting at

to a Bohemia Scenic

Countryside

*Castle Kost*

9.00 a.m.