IInd INTERNATIONAL SEMINAR
ON HIGH RESOLUTION INFRARED SPECTROSCOPY, PRAGUE
September 4 - 8, 1972

Program of Sessions
IInd INTERNATIONAL SEMINAR
ON HIGH RESOLUTION INFRARED SPECTROSCOPY, PRAGUE
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Organizing Committee:
D. Papoušek (Chairman)
Z. Cihla, M. Horák, J. Pitrová (Secretary), R. Sovička,
J. M. R. Stone, V. Špirko
IIInd International Seminar
on High Resolution Infrared Spectroscopy, Prague
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Program of Sessions

Monday, September 4

Opening Ceremony 9.00 a.m.

Morning Session: (A) General Theory
(Chairman - Prof. I. Kovács)

A 1. G. Amat (Faculté des sciences de Paris, Laboratoire
de spectroscopie moléculaire, France):
"Vibration-Rotation Line Intensities" (invited paper)
10.00 - 10.45

A 2. A. Chedin and Z. Cihla (Faculté des sciences de Paris,
Laboratoire de spectroscopie moléculaire,
France and J. Heyrovský-Institute of Physical
Chemistry and Electrochemistry, Czechoslovak
Academy of Sciences, Prague, Czechoslovakia):
"Algebraic Manipulations with Computers: Recent Progress in the Field of Molecular Spectroscopy"
11.00 - 11.30

A 3. Z. Cihla and A. Chedin (J. Heyrovský-Institute of Physical
Chemistry and Electrochemistry, Czechoslovak
Academy of Sciences, Prague, Czechoslovakia and Faculté des sciences de Paris,
Laboratoire de spectroscopie moléculaire,
France):
"Manipulations algébriques de polynomes non-
commutatifs"
11.35 - 12.00
**Afternoon Session: (B) Experimental Methods of High Resolution Spectroscopy**

(Chairman - Dr. W.B. Olson)

B 1. K. Narahari Rao (The Ohio State University, Department of Physics, Columbus, U.S.A.):

"Aspects of Research in Infrared Spectroscopy at the Ohio State University" (invited paper)

2.00 - 2.45

B 2. C.P. Courtoy and J. Warland (Faculté universitaire, Département de physique, Namur, Belgique):

"High Resolution Infrared Spectra with a 'Grille' Spectrometer"

3.00 - 3.25

B 3. K.D. Möller, A. Pluchino and C. Belorgeot (Department of Physics, Fairleigh Dickinson University, Teaneck N.J., U.S.A.):

"Far Infrared Fourier Transform Spectrometer"

3.30 - 3.55

**Afternoon Session: (C) General Theory**

(Chairman - Prof. G. Amat)

C 1. E.K. Gore (Max-Planck-Institut für Physik und Astrophysik, München, B R D):

"On the Use of Contact Transformations in Closed Form in the Theory of Vibration-Rotation Spectra"

4.10 - 4.30


"The Possibility of an Optimal Choice for the Semiempirical Parameters in the Calculation of Centers and Intensities of Vibration-Rotational Lines of $H_2O$ Molecules"

4.35 - 5.00
Tuesday, September 5

Morning Session: (D) Molecules with Large Amplitude Motions
(Chairman - Dr. J.K.C. Watson)

D 1. P. Bunker (National Research Council of Canada, Division of Pure Physics, Ottawa, Canada):
"The Vibration-Rotation Problem in Triatomic Molecules" (invited paper) 9.00 - 9.30

D 2. J.M.R. Stone, V. Špirko and D. Papoušek (J. Heyrovský-Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague, Czechoslovakia):
"A New Vibration-Inversion-Rotation Hamiltonian for Ammonia" 9.45 - 10.15

"Millimeter Wave Spectra and Structure of DCNO and HCNO in Vibrationally Excited States" (invited paper) 10.20 - 10.50

D 4. B.P. Winnewisser (Institut für physikalische Chemie, Kiel, B D R):
"Far Infrared Spectra of HCNO and DCNO" 11.15 - 11.40

D 5. L. Sztraka (Department of Physical Chemistry, Technical University, Budapest, Hungary):
"The Internal Rotation Problem in the Hydrazine Molecule" 11.50 - 12.15

Afternoon Session: (E) Molecules with Large Amplitude Motions
(Chairman - Dr. P. Bunker)

E 1. J.W.C. Johns, J.M.R. Stone and G. Winnewisser (National Research Council of Canada, Division of Physics, Ottawa, Canada; J. Heyrovský-Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague, Czechoslovakia and Max-Planck-Institut für Radioastronomie, Bonn, B R D):
"The Infrared and Millimeterwave Spectrum of Ketene" 2.00 - 2.15
E 2. L. Nemes (Central Research Institute for Chemistry, Hungarian Academy of Sciences, Budapest, Hungary):
"The Analysis of the K-Structure of ν₇ and ν₉ of Ketene"
2.20 - 2.35

E 3. G. Winnewisser (Max-Planck-Institut für Radioastronomie, Bonn, B.R.D.):
"Millimeter Wave Spectra of HSSH and DSSD in Vibrationally Excited States"
2.40 - 3.00

E 4. R. Anttila and M. Huhantti (Department of Physics, University of Oulu, Finland):
"Rotation-Vibration Bands of DCCF"
3.05 - 3.25

E 5. D. Papoušek and V. Danielis (J. Heyrovský-Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague, Czechoslovakia):
"Vibration- Rotation-Contortion Hamiltonian for Molecules with Several Large Amplitude Motions"
3.30 - 3.55

Afternoon Session: (F) Force Constant Calculations
(Chairman - Dr. M. Winnewisser)

F 1. I.M. Mills (Department of Chemistry, University of Reading, England):
"Anharmonic Force Constant Calculations" (invited paper)
4.15 - 4.45

"Ab Initio Calculation of Force Constants for Nitrogen Fluorides and Oxyfluorides"
5.00 - 5.25
**Wednesday, September 6**

**Morning Session:** (G) Analysis of High-Resolution Infrared Spectra

(Chairman - Prof. K. Narahari Rao)

"Perturbation Allowed Transitions and New Measurements of the $\nu_1$ and $\nu_3$ Bands of AsH$_3$"

9.00 - 9.25

G 2. K. Sarka (Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Czechoslovakia):
"Perturbation Allowed Transitions and Determination of $\Lambda_0$"

9.30 - 9.55

G 3. D. Van Lerberghe (Université de Louvain, Institut de physique corpusculaire, Ottignies, Belgique):
"Infrared High Resolution Study of C$_2$H$_4$ between 1800 and 6200 cm$^{-1}$ and Some New Data on Isotopic Derivatives"

10.10 - 10.35

G 4. C. di Lauro and C. Festa (Istituto chimico, Università di Napoli, Italy and Istituto di chimica fisica, Università di Pisa, Italy):
"Fermi Resonance in the System $2\nu_4$, $\nu_4 + 3\nu_6$ of Methyl Chloride"

10.50 - 11.15

G 5. G. Balquet and C.P. Courtoy (Faculté universitaire, Département de physique, Namur, Belgique):
"Molecular Constants of $^{13}\text{C}-^{32}\text{S}_2$"

11.20 - 11.45

**Afternoon Session:** (H) Analysis of High-Resolution Infrared Spectra

(Chairman - Dr. M. Aliiev)

H 1. C. Camy-Peyret and J.M. Fland (Faculté des sciences de Paris, Laboratoire de spectroscopie moléculaire, Paris, France):
"High Resolution Infrared Spectra of Some H$_2^{16}$O Vibrational Bands"

2.00 - 2.25
H 2. G. Steenbeckeliers, J. Bellet and A. Feyt (Institut de physique nucléaire de Lille-Annappes, France):
"High Resolution Infrared and Microwave Spectra of Stable and Radioactive Isotopic Species of Water"
2.30 - 2.55

H 3. H. Hollenstein and Hs.H. Günther (Swiss Federal Institute of Technology, Physico-Chemical Laboratory, Zurich, Switzerland):
"Coriolis Interaction in Acetaldehyde. Computer Simulated Band Contours"
3.00 - 3.25

H 4. A. Ruoff and R. Anttila (Sektion für Schwingungsspektroskopie, Universität Ulm, B R D and Physikalisches Institut, Universität Oulu, Finland):
"Bendenkontursimulation des Kombinationstones \(v_1 + v_3\) von HCCl_3"
3.45 - 4.10

H 5. F. Winther (Abteilung für chemische Physik, Institut für physikalische Chemie, Kiel, B R D):
"Far Infrared Rotation-Vibration Bands"
4.15 - 4.40

H 6. C. Betrencourt and M. Morillon (Laboratoire d'infra-rouge, Chimie physique, Faculté des sciences de Paris, Orsay, France):
"Etude de la bande 2\(\nu_2\) du bromure de méthyle vers 2600 \(\text{cm}^{-1}\)"
4.45 - 5.10

Thursday, September 7

Morning Session: (I) General Theory
(Chairman - Dr. J.T. Hougen)

I 1. I. Kovács (Department of Atomic Physics, Polytechnical University, Budapest, Hungary):
"Centrifugal Distortions and Multiplet Structure (with an application to the doublet terms)" (invited paper)
9.00 - 9.45

I 2. J.K.G. Watson (Department of Physics, The Ohio State University, Columbus, U.S.A.):
"Forbidden Rotational Spectra" (invited paper)
10.00 - 10.30
I 3. M. Aliev (Institute for Spectroscopy, Academy of Sciences of the USSR, Moscow):

"Centrifugal Distortion in Polyatomic Molecules" (invited paper) 10.45 - 11.10

I 4. M.D. Kusanova (Physics Department, University of Sofia, Bulgaria):

"General Method for Theoretical Definition of the Molecular Parameters" 11.15 - 11.40

I 5. A. Müller, N. Mohan and K.H. Schmidt (Lehrstuhl für anorganische Chemie der Universität Dortmund, B R D):

"Studies of the Mass Effect on Molecular Constants by Using Perturbation Theory" 11.45 - 12.10

Afternoon Session: (J) Excursion to the Infrared Laboratory of the Institute of Physical Chemistry and Electrochemistry

J 1. R. Sůvicka, M. Holub and M. Matucha (Czechoslovak Academy of Sciences, J. Heyrovský-Institute of Physical Chemistry and Electrochemistry, Prague, Czechoslovakia):

"Demonstration of the High Resolution Infrared-Grating Spectrometer of the Institute of Physical Chemistry and Electrochemistry in Prague"

Starting at 2.00 p.m.

Friday, September 8

Morning Session: (K) Microwave Studies, Laser Spectroscopy
(Chairman - Prof. I.M. Mills)

K 1. A.F. Krupnov (Radiophysical Research Institute, Gorky, USSR):

"Millimeter and Submillimeter Spectroscopy of Gases over a Wide Region" (invited paper) 10.00 - 10.30
"Reinterpretation of Molecular Beam Hyperfine Data for $^{14}$NH$_3$ and $^{15}$NH$_3$"
10.35 - 11.00

K 3. L.M. Imanov (Institut fiziki AN Az.SSR, Baku, USSR):
"Investigation of the Microwave Spectra of Alcohols"
11.05 - 11.30

"An Interesting Example of Hund's Coupling Case (c) in HgAr"
11.45 - 12.10

K 5. V.E. Zuev, V.P. Lopasov and A.P. Godlevsky (Institute of Atmospheric Optics, Tomsk, USSR):
"High Resolution High-Speed Laser Spectrometry of Gaseous Media"
12.15 - 12.45

Afternoon Session: (L) Force Constant Calculation

(Chairman - Prof. W. Sawodny)

L 1. G. Streuy, A.R. Hoy and I.M. Mills (University of Reading, Department of Chemistry, Reading, England):
"Least Squares Adjustment of Anharmonic Potential Constants: Application to Small Molecules"
2.35 - 3.00

L 2. A. Alix (Laboratoire de recherches optiques, Faculté des sciences, Reims, France):
"On the Iteration Solution of Force Constants"
3.05 - 3.30

"Force Constant Calculations of Simple Oxygen and Sulphur Compounds of Chromium, Molybdenum and Rhenium from $^{16}$O, $^{50}$Cr, $^{53}$Cr, $^{92}$Mo, $^{100}$Mo Isotope Shifts"
3.35 - 4.00
L 4. H. Schulze, N. Weinstock and A. Müller (Anorganisch-Chemisches Institut, Göttingen, B R D):
"Kraftkonstanten von \( \text{PO}_4^{3-}, \text{SO}_4^{2-}, \text{ClO}_4^{-}, \text{SeO}_4^{2-} \)
und \( \text{BrO}_4^{-} \) aus Raman-Intensitäten"

4.05 - 4.30