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**IVth INTERNATIONAL SEMINAR ON HIGH RESOLUTION
INFRARED SPECTROSCOPY, LIBLICE NEAR PRAGUE,
SEPTEMBER 6 - 10, 1976**

**Program of Sessions
Abstracts of Papers**

**The J. Heyrovský Institute of Physical Chemistry
and Electrochemistry, Czechoslovak Academy of
Sciences**

Czechoslovak Spectroscopic Society

IVth INTERNATIONAL SEMINAR ON HIGH RESOLUTION
INFRARED SPECTROSCOPY, LIBLICE NEAR PRAGUE,
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Program of Sessions

Monday, September 6

Opening Ceremony 9.00 a.m.

Morning Session (Chairman - J.T. Hougen)

A1. K. Narahari Rao (Department of Physics, The Ohio State University, Ohio, U.S.A.):

"Research in High Resolution Infrared Spectroscopy - An Overview"

9.15 - 10.00 a.m.

Intermission 10.00 - 10.15 a.m.

A2. V.S. Letochov (Institute for Spectroscopy, Academy of Sciences, Moscow, U.S.S.R.):

"Selective Infrared Laser Photophysics and Photochemistry of Molecules"

10.15 - 11.00 a.m.

Intermission 11.00 - 11.15 a.m.

A3. L. Henry (Laboratoire de Spectrométrie Moléculaire, Université de Paris VI, France):

"Laser Spectroscopy"

11.15 - 12.00 a.m.

in front of castle

photograph = free

pay today upstairs.

Afternoon Session (Chairman - K. Narahari Rao)

JKGW at 1:30 pm

B1. J.T. Hougen (Molecular Spectroscopy Section, National Bureau of Standards, Washington, U.S.A.):

"Calculation of Vibrational Level Populations in Multiphoton Absorption Processes" (Invited lecture)

2.00 - 2.25 p.m.

B2. R.S. McDowell, H.W. Galbraith, B.J. Krohn, and C.D. Cantrell (University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico, U.S.A.) and E.D. Hinkley (MIT Lincoln Laboratory, Lexington, Massachusetts 02171, U.S.A.):

"Diode Laser Spectroscopy and Vibration-Rotation Assignments of SF₆"

2.30 - 2.50 p.m.

B3. A. Mantz (Digilab, Cambridge, Massachusetts, U.S.A.):

"Time Resolved Spectroscopy" (invited lecture)

2.55 - 3.25 p.m.

Intermission 3.30 - 3.45 p.m.

- B4. A.R.H. Cole (The University of Western Australia, School of Chemistry, Perth, Australia):
"The Revised IUPAC Infrared Calibration Tables"
3.45 - 4.05 p.m.
- B5. P. Varanasi (Laboratory for Planetary Atmospheres Research, College of Engineering and Applied Science, State University of New York, Stony Brook, U.S.A.):
"Collision-Broadened Line Measurements on Atmospheric Molecules"
4.10 - 4.30 p.m.
- B6. A. Picard (Laboratoire Infrarouge, Université Paris XI, Orsay, France):
"Vibrational Relaxation of N_2O Excited by Activated N_2^* "
4.35 - 4.55 p.m.
- B7. H. Finsterhölzl, J.G. Hochenbleicher, K. Altman, and G. Stray (Sektion Physik, Universität München, B.R.G.):
"Intensity Distribution in Pure Rotational Raman Spectra of Linear Molecules in the Ground and Excited Vibrational Π States"
5.00 - 5.20 p.m.

Tuesday, September 7

Morning Session (Chairman - L. Henry)

Laser Spectroscopy, Saturated Absorption

- C1. C. Betrencourt-Stirnermann and J.C. Deroche (Laboratoire d'Infrarouge, Orsay, France):
"Assignment of CH_3Br Transitions Pumped by CO_2 Laser"
9.00 - 9.20 a.m.
- C2. M. Ouhayon⁽¹⁾, J. Bordé⁽²⁾, and C. Bordé⁽¹⁾
⁽¹⁾ Laboratoire de Physique des Lasers, Université de Paris-Nord, Saint-Denis, France
⁽²⁾ Laboratoire de Physique Moléculaire et d'Optique Atmosphérique, C.N.R.S., Orsay, France):
"Vibrational Dependence of the Hyperfine Quadrupole Constant in NH_3 Observed by Saturated Absorption Spectroscopy"
9.25 - 9.40 a.m.

- C3. S.N. Murzin and V.G. Koloshnikov (Institute of Spectroscopy, Academy of Sciences, Moscow, U.S.S.R.):
"Transient Saturation in the ND_3 Inversion Spectrum" 9.45 - 10.15 a.m.
- C4. B.D. Osipov (Institute of Spectroscopy, Academy of Sciences, Moscow, U.S.S.R.):
"Double Resonance Study of Hyperfine Structure of the $\text{CH}_3\text{I}^{127}$ Molecule" 10.20 - 10.35 a.m.
Intermission 10.40 - 10.55 a.m.
- C5. H. Jones and F. Kohler (Universität Ulm, Med.-Naturwiss. Hochschule, Ulm, B.R.D.):
"Laser-Microwave Double Resonance and Double Photon Spectroscopy in Some Linear Molecules" 10.55 - 11.10 a.m.
- C6. F. Kohler and H. Jones (Universität Ulm, Med.-Naturwiss. Hochschule, Ulm, B.R.D.):
"Laser-Infrared Double Resonance Experiments in Some Symmetric-Top Molecules" 11.10 - 11.25
- C7. W. Radloff (Central Institute of Optics and Spectroscopy, Academy of Sciences of the GDR, Berlin, GDR):
"Isotope Detection by High Resolution Laser Spectroscopy" 11.35 - 11.50
- C8. E. Meisel (Central Institute of Optics and Spectroscopy, Academy of Science of the GDR, Berlin, GDR):
"Lamb-Dip Spectroscopy with the CO_2 Laser" 11.55 - 12.10 a.m.
- C9. M. Dubs (Federal Institute of Technology, Zürich, Switzerland):
NOT GIVEN "Diode Laser Spectra of Matrix Isolated Molecules" 12.15 - 12.30 a.m.

J. Balica

Afternoon Session (Chairman - K. Yamada)

Submillimeter and Microwave Spectroscopy

- D1. A.F. Krupnov and A.V. Burenin (Radiophysical Research Institute, Gorky, U.S.S.R.):
"Submillimeter Microwave Spectroscopy: Theory and Experiment" (invited lecture)
2.00 - 2.30 p.m.
- D2. J. Bellet, D. Dangoisee, A. Deldalle and J.P. Springard (Laboratoire de Spectroscopie Hertzienne U.E.R. de Physique, Université de Lille, France):
"Accurate Measurement of the Formic Acid Submillimeter Laser CW Lines"
2.35 - 2.55 p.m.
- D3. D. Boucher, J. Burie, J. Demaison, A. Dubrulle and G. Journal (Laboratoire de Spectroscopie Hertzienne, Université des Sciences et Techniques de Lille, France):
"High Resolution Rotational Spectra of Methyl Halides Using a Molecular Beam Spectrometer"
3.00 - 3.15 p.m.
- Intermission 3.20 - 3.35 p.m.
- D4. I. Botskor and H.D. Rudolph (Abteilung Physikalische Chemie, Universität Ulm, B.R.D.):
"Microwave Studies of Rotational Isomerism in Allylamine: The N-cis, Lone Electron Pair-Gauche Isomer"
3.35 - 3.50 p.m.
presented by Creswell
- D5. E.F. Pearson and B.P. Winniewisser (Physikalisch-Chemisches Institut der Justus Liebig-Universität, Giessen, B.R.D.):
"Vibration-Rotation Interaction in the Alkali Hydroxides"
3.55 - 4.15 p.m.
- D6. L. Nemes (Central Research Institute for Chemistry, Hungarian Academy of Science, Budapest, Hungary):
"On the τ -Defect"
4.20 - 4.35 p.m.

Discussion of J Mol. Spec. policies 4:45 pm
Wednesday, September 8

Morning: Sight-seeing Tour

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

Because of time shortage, during the excursion
will be presented a lecture:

R. Sovička, D. Papoušek, V. Špirko, M. Horák, M. Matucha
and M. Holub:

"High Resolution Spectra of CH_3CN , $2\nu_5$ and
 $\nu_1 + \nu_5$ Bands"

Thursday, September 9

Morning Parallel Session (Chairman - M.R. Aliev)

Spherical Top Molecules

E1. J. Moret-Bailly (Laboratoire de Spectromie Moléculaire,
Université de Dijon, France):

"New Applications of Group Theory in the Study
of Spherical Top Molecules" (invited lecture)

9.00 - 9.40 a.m.

E2. K. Fox (Department of Physics, University of Tennessee,
Knoxville, Tennessee, U.S.A.):

"Recent Developments in High-Resolution Spectro-
scopy of Spherical-Top Molecules" (invited
lecture)

9.45 - 10.30 a.m.

E3. J.P. Champion (Laboratoire de Spectromie Moléculaire,
Université de Dijon, France):

"Relatione entre les différents schémas de
couplage rotation-vibration dans l'étude des
bandes de vibration-rotation des molécules
du type XY_4 "

10.35 - 10.50 a.m.

Intermission 10.55 - 11.10 a.m.

E4. G. Pierre (Laboratoire de Spectromie Moléculaire,
Université de Dijon, France):

"Etude des bandes harmoniques $2\nu_3$ et $2\nu_4$
des molécules XY_4 . Application à $2\nu_4$
de CH_4 et $2\nu_3$ de SiH_4 "

11.10 - 11.25 a.m.

E5. F. Michelot (Laboratoire de Spectromie Moléculaire,
Université de Dijon, France):

"Doubly Degenerate Vibrational Levels for
Spherical Tops: A General Study Using the
 $\text{O}(3)$ Teneor Formalism"

11.30 - 11.45 a.m.

- E6. M.C.L. Gerry, I. Ozier, R.H. Kagann and R.M. Lee
(Department of Chemistry and Department of
Physics, The University of British Columbia,
Vancouver, Canada):
"The Microwave Distortion Moment Spectra of a
Series of Tetrahedral Molecules"
11.50 - 12.10 a.m.

Morning Parallel Session (Chairman - A. Mantz)

Fourier Transform Spectroscopy

- EE1. C. Amiot (Laboratoire de Physique Moléculaire et
d'Optique Atmosphérique, C.N.R.S., Orsay,
France):
"High Resolution Fourier Spectra of Five
Isotopic Species of N₂O. Potential Energy
Function"
9.00 - 9.20 a.m.
- EE2. A.A. Balashov, V.S. Bukreev, V.A. Vagin, N.G. Kultapin,
I.N. Nesteruk, and G.N. Zhizhin (Institute of Spectro-
scopy, Academy of Sciences, Moscow, U.S.S.R.):
"Fourier-Transform Spectrometer for 0.6 - 100 μ m
with Resolution 0.01 - 0.005 cm⁻¹"
9.25 - 9.40 a.m.
- EE3. A.A. Balashov, V.S. Bukreev, V.A. Vagin, E.B. Perminov,
and G.N. Zhizhin (Institute of Spectroscopy, Academy
of Sciences, Moscow, U.S.S.R.):
"Infrared Luminescence Studies of Dy²⁺-Doped
CaF₂ at Helium Temperature on High Resolution
Fourier Spectrometer" 9.45 - 10.00 a.m.
Intermission 10.05 - 10.20 a.m.
- EE4. V.A. Ageikin and V.G. Koloshnikov (Institute of
Spectroscopy, Academy of Sciences, Moscow,
U.S.S.R.)
"Scanning Fabry-Perot Interferometers SI-1 and
SKI-1 for the 5-30 μ m Region"
10.20 - 10.35 a.m.
- EE5. S. Gerstenkorn and P. Luc (Laboratoire Aimé-Cotton-
C.N.R.S. II, Orsay, France): 91405 ORSAY
"Rotational Analysis of the 5350 Å Band of
Iodine by Means of Fourier Transform Spectro-
scopy"
10.40 - 10.55 a.m.

- EE6. G. Fenske (Zentralinstitut für Optik und Spektroskopie, Akademie der Wissenschaften der DDR, Berlin, D.D.R.):
"Generalizing of Instrument Profile in Fourier Spectroscopy and Application on High Resolution"
11.00 - 11.15 a.m.

Afternoon Session (Chairman - J. Bordé)

Theory and Analysis of the High Resolution Infrared Spectra

- F1. D. Van Lerberghe (Institut de Physique, Université de Louvain, Belgique):
"Six Years to Know Something About Six Atoms Molecules. Study of Six Isotopic Species of Ethylene" (invited lecture)
2.00 - 2.20 p.m.
- F2. M.R. Aliev (Institute of Spectroscopy, Academy of Sciences, Moscow, U.S.S.R.):
"Forbidden Rotational Spectra of Nonpolar Molecules in Degenerate Electronic States" (invited lecture)
2.25 - 2.45 p.m.
- F3. A. Barbe⁽¹⁾, C. Secroun⁽¹⁾, P. Jouve⁽¹⁾, B. Duterage⁽²⁾, N. Monnanteuil⁽²⁾, J.C. Depannemaecker⁽²⁾, J. Bellat⁽²⁾, P. Pinson⁽³⁾ ((1) Laboratoire de Physique Moléculaire, C.N.R.S., Faculté des Sciences, Reims, France, (2) Laboratoire de Spectroscopie Hertzienne, C.N.R.S., Université de Lille, France, (3) Laboratoire d'Infrarouge, C.N.R.S., Université de Paris XI, Orsay, France):
"Spectres haute resolution infrarouge et micro-onde de la bande ν_3 de l'ozone"
2.50 - 3.05 p.m.
- F4. M. Betrençourt and M. Morillon-Chapey (Laboratoire d'Infrarouge, Campus d'Orsay, France):
"Accidental and Essential Resonances in the Spectrum of CH_3F Near 2500 cm^{-1} "
3.10 - 3.25 p.m.
Intermission 3.30 - 3.45 p.m.
- F5. M.Y. Chan and P.M. Parker (Department of Physics, Michigan State University, Michigan, U.S.A.):
"Centrifugal Distortion Coefficients of $^{16}\text{O}_3$ "
3.50 - 4.05 p.m.

- F6. J.L. Destombes, Mme C. Marliere, and G. Journal
(Laboratoire de Spectroscopie Hertzienne de
l'Université des Sciences et Techniques de
Lille, France):

"A Model for the Interpretation of UV, IR
and Microwave Spectra of the OH Radical"
4.10 - 4.25 p.m.

Friday, September 10

Morning Session (Chairman - G. Strey)

Molecules with Large Amplitude Motions

- G1. K. Yamada⁽¹⁾, M. Winnewisser⁽¹⁾, L.B. Szalanek⁽²⁾ and
M.C.L. Gerry⁽²⁾ ⁽¹⁾Physikalisch-Chemisches Institut
des Justus Liebig-Universität, Giessen, B.R.D.
⁽²⁾Department of Chemistry, The University of
British Columbia, Vancouver, Canada):
"The Vibration-Rotation Interactions Among the
Three Bending Modes of HNC0 and HNCS Studied
by Microwave and Millimeterwave Spectra"
9.00 - 9.20 a.m.
- G2. R.A. Creswell, E.F. Pearson, M. Winnewisser, and
G. Winnewisser (Physikalisch-Chemisches Institut der
Justus Liebig-Universität, Giessen, B.R.D.):
"Millimeter Wave Spectrum of Hydrogen Isocya-
nide, HNC, and Its Astrophysical Implications"
9.25 - 9.40 a.m.
- G3. I. Boháček, V. Danielis, D. Papoušek, and V. Špirko
(The J. Heyrovský Institute of Physical Chemistry
and Electrochemistry, Czechoslovak Academy of
Sciences, Prague, Czechoslovakia):
"Inverse" Eigenvalue Problem for the Schrödinger
Equation with a Singularity-Determination of
the Potential Function in Quasilinear Molecules"
9.45 - 10.00 a.m.
- G4. F. Winther (Abteilung Chemische Physik, Institut für
Physikalische Chemie, Universität Kiel, B.R.D.):
"The Pure Rotational Spectrum of H₂¹⁸O and
H₂¹⁷O in the Far Infrared"
10.05 - 10.20 a.m.

Intermission

- G5. H. Hollenstein and F. Winther (Eidgenössische Technische Hochschule Zürich, Laboratorium für Physikalische Chemie, Zürich, Schweiz, and Institut für Physikalische Chemie der Universität Kiel, Kiel, B.R.D.):
 "Analysis of the "K-Structure" of the Torsional Fundamental of Acetaldehyde"
 10.40 - 10.55 a.m.
- G6. J. Mink⁽¹⁾, M. Gál⁽¹⁾ and L. Nemes⁽²⁾ (⁽¹⁾ Institute of Isotopes of the Hungarian Academy of Sciences, Budapest, Hungary, ⁽²⁾ Central Research Institute for Chemistry of the Hungarian Academy of Sciences, Budapest, Hungary):
 "Rotational Analysis of the Far-Infrared Spectra of cis-HNSO"
 11.00 - 11.15 a.m.
- G7. J. Mink, G. Kemény, and R. Kremo (Institute of Isotopes of the Hungarian Academy of Sciences, Budapest, Hungary):
 Rotational-Vibrational Infrared and Raman Spectra of Dimethylmercury"
 11.20 - 11.45 a.m.

Morning parallel sessions

Afternoon Session (Chairman - J. Moret-Bailly)

Potential Functions of Polyatomic Molecules, Miscellaneous

- H1. N. Husson and I. Jobard (C.N.R.S., Batiment 221 (Campus d'Orsay), 91405 Orsay, France):
 Critical Analysis of Series Expansions of the Potential Energy Function of CO₂. Potential Energy Contour Maps"
 2.00 - 2.20 p.m.
- H2. V. Špirko (The J. Heyrovský Institute of Physical Chemistry and Electrochemistry, Czechoslovak Academy of Sciences, Prague, Czechoslovakia):
 "A Few Remarks Concerning the Application of the Polynomial Expansion Technique in the Theory of Vibration-Rotation Spectra"
 2.20 - 2.45 p.m.
- H3. P. Henning, W.P. Kraemer, and G.H. Dicrcksen (Max Planck Institut für Physik und Astrophysik, München, B.R.D.):
 "Calculation of Rotational Frequencies of Small Linear Radicals From Ab Initio CI-Data; HCN (for comparison); HNC, HCO⁺, HOC⁺, HNN⁺"
 2.45 - 3.00 p.m.

- H4. V. Kvasnička (Department of Mathematics, Faculty of Chemistry, Slovak Technical University, Bratislava, Czechoslovakia):
"The Many-Body Diagrammatic Perturbation Theory of Rotation-Vibration Spectra"
3.05 - 3.20 p.m.
- Intermission 3.25 - 3.40 p.m.
- H5. K. Sárka⁽¹⁾ and S.A. Kirillov⁽²⁾ (⁽¹⁾Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Czechoslovakia, ⁽²⁾Institute of General and Inorganic Chemistry, Ukrainian Academy of Sciences, Kiev, U.S.S.R.):
"Broadening of Vibrational Lines in Liquids Caused by Short Range Interactions"
3.40 - 3.55 p.m.

Post Deadline Papers

- A. Fayt and R. Vandenhaute (University of Louvain, Institut de Physique Chemin du Cyclotron, Louvain, Belgium):
" Rovibrational Analysis of the Principal Isotopic Species of Carbonyl Sulphide"
- A.D. Bykov, Yu.S. Makushkin, and O.N. Ulenikov (Institute of Atmospheric Optics, Academy of Sciences, Siberian Branch, Tomsk, U.S.S.R.):
"Investigation of Isotopic Dependence of Parameter in Polyatomic Molecules"
- Yu.S. Makushkin and Vl.G. Tyuterev (Institute of Atmospheric Optics, Academy of Sciences, Siberian Branch, Tomsk, U.S.S.R.):
" Effective Hamiltonians Having Applications in the Theory of Vibrational-Rotational Spectra"
- ✓ M. Römheld (Abteilung für Physikalische Chemie, Universität Ulm, B.R.D.):
"Stark Spectroscopy of the ν_4 Vibration-Rotation Band of Methyl Isocyanide Using CO_2 and N_2O Lasers"
- ✓ J.K.G. Watson (Chemistry Department, The University Southampton, England):
"Higher-Order Vibrational-Rotational Perturbation Theory"
- J. Drozdzyński (Institute of Chemistry, University of Wrocław, Poland):
"Absorption Spectra and Energy Level Scheme of Uranium $+3/$ "
- ✓ J. Galica, S. Gierszal, E. Miś-Kuźmińska and W. Prussak (Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland):
"Frequency Measurements of Hyper-fine Structure Lines for Inversion Transition of the Ammonia Molecule for the States $J = K = 2 - 8$ "

The Meeting will end on Friday, September 10th in the afternoon. Transports from Liblice will start at 5.00 p.m. Should your travel plans require a hotel reservation in Prague after the Meeting, please, contact our Travel Agency ČEDOK, Congress Center/347, Přikopy 18, 111 35 Prague 1. Unfortunately, it is impossible for the Institute to secure any accomodation.

The Organizing Committee also cannot secure any transport of participants in Prague before or after the Conference except the transport from Prague to Liblice and back, and the excursion to the Infrared Lab.

SOCIAL PROGRAM

Monday:

Coctail Party 7.00 p.m.

Tuesday:

Barbecue (Banquet) 7.30 p.m.

Wednesday:

Sight-Seeing Tour to a Bohemia
Scenic Countryside 9.00 a.m.

Organizing Committee:

D.Papoušek (Chairman), V.Špirko (Deputy Chairman),
I.Boháček, V.Daniclis, H.Holub (Technician),
M.Horák, R.Sovička, P.Engst, V.Zedlerová (Secretary),
L.Bureš (Economic)

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