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**MOLECULAR
SPECTROSCOPY**

THE OHIO STATE UNIVERSITY

June 15-19, 1987

UNDER THE SPONSORSHIP OF
THE DEPARTMENT OF PHYSICS
THE DEPARTMENT OF CHEMISTRY
THE GRADUATE SCHOOL
OF THE UNIVERSITY
AND
THE U.S. ARMY RESEARCH OFFICE
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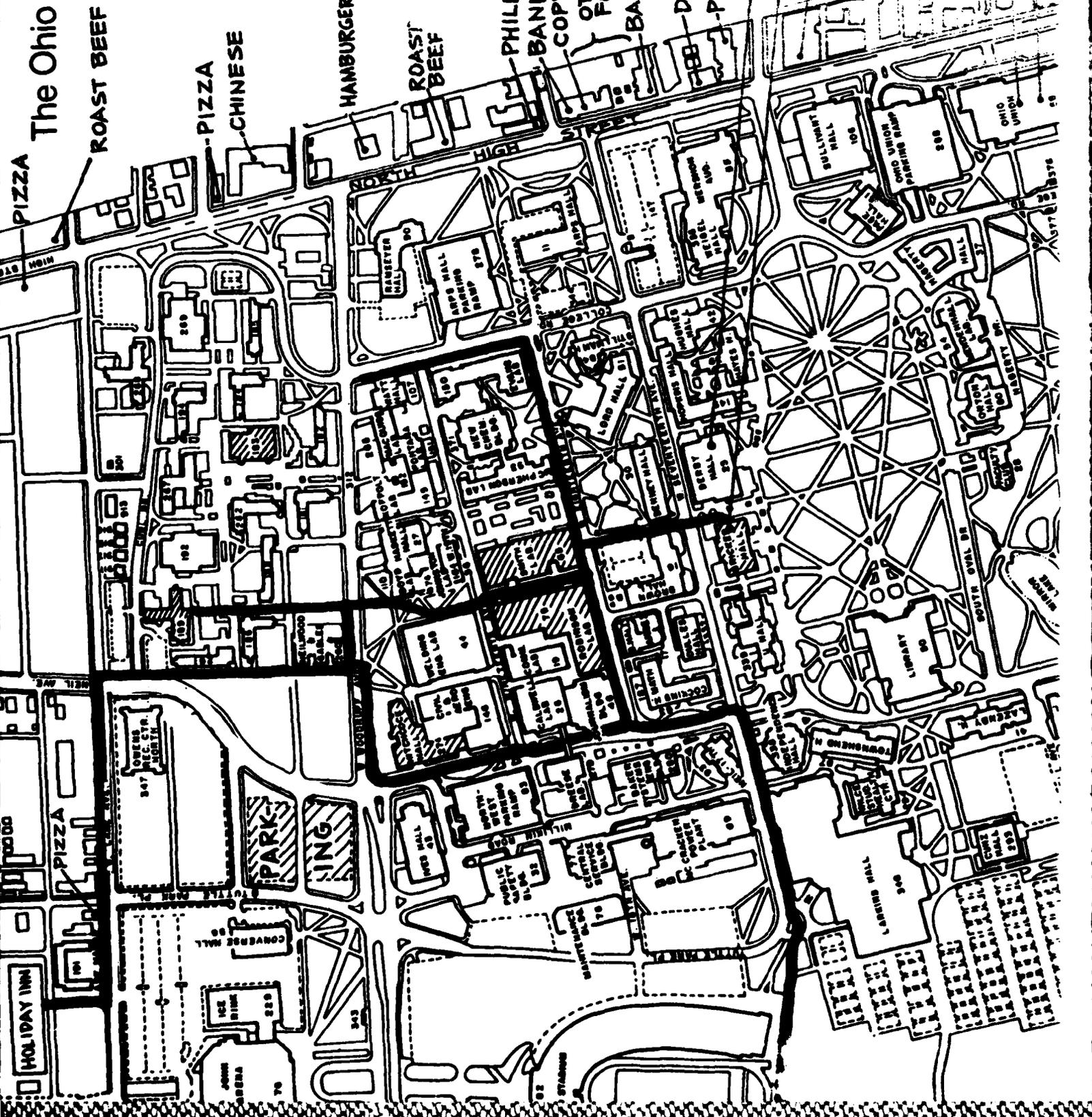
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REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION Unclassified			1b. RESTRICTIVE MARKINGS			
2a. SECURITY CLASSIFICATION AUTHORITY			3. DISTRIBUTION / AVAILABILITY OF REPORT Approved for public release; Distribution unlimited.			
2b. DECLASSIFICATION / DOWNGRADING SCHEDULE						
4. PERFORMING ORGANIZATION REPORT NUMBER(S)			5. MONITORING ORGANIZATION REPORT NUMBER(S) AFOSR-TR-87-1266			
6a. NAME OF PERFORMING ORGANIZATION Ohio State University Research Foundation		6b. OFFICE SYMBOL (if applicable)	7a. NAME OF MONITORING ORGANIZATION AFOSR/NC			
6c. ADDRESS (City, State, and ZIP Code) Department of Physics Columbus, OH 43212-1994			7b. ADDRESS (City, State, and ZIP Code) Building 410 Bolling AFB, DC 20332-6448			
8a. NAME OF FUNDING / SPONSORING ORGANIZATION AFOSR		8b. OFFICE SYMBOL (if applicable) NC	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER AFOSR-86-0065			
8c. ADDRESS (City, State, and ZIP Code) Building 410 Bolling AFB, DC 20332-6448			10. SOURCE OF FUNDING NUMBERS			
			PROGRAM ELEMENT NO. 61102F	PROJECT NO. 2310	TASK NO. A1	WORK UNIT ACCESSION NO.
11. TITLE (Include Security Classification) Forty-Second Symposium on Molecular Spectroscopy						
12. PERSONAL AUTHOR(S) Dr. K. Narahari Rao						
13a. TYPE OF REPORT Interim		13b. TIME COVERED FROM 6/15/87 TO 6/19/87		14. DATE OF REPORT (Year, Month, Day)		15. PAGE COUNT
16. SUPPLEMENTARY NOTATION						
17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)			
FIELD	GROUP	SUB-GROUP				
19. ABSTRACT (Continue on reverse if necessary and identify by block number) The 42nd Symposium on Molecular Spectroscopy was convened at Ohio State University during the period 15-19 June 1987. Over 300 scientists attended, representing research organizations from the U.S. and fourteen foreign countries. Topical areas included electronic characteristics of molecules, energy transfer, infrared and microwave spectra, liquid and solid state phenomena, laser spectra, Raman spectra, molecular beams, vibrational analysis, and experimental techniques. As planned, special emphasis was placed on the spectroscopy of van der Waals molecules, and there was a special session on probing and modeling the earth's atmosphere. ↑						
20. DISTRIBUTION / AVAILABILITY OF ABSTRACT <input checked="" type="checkbox"/> UNCLASSIFIED/UNLIMITED <input checked="" type="checkbox"/> SAME AS RPT <input type="checkbox"/> DTIC USERS				21. ABSTRACT SECURITY CLASSIFICATION Unclassified		
22a. NAME OF RESPONSIBLE INDIVIDUAL JAMES P. KOERMER, Lt Col, USAF			22b. TELEPHONE (Include Area Code) (202) 767-4960		22c. OFFICE SYMBOL NC	

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AN IMPORTANT ANNOUNCEMENT

THE 43RD MOLECULAR SYMPOSIUM WHICH WILL TAKE PLACE AT THIS UNIVERSITY IN A YEAR FROM NOW (JUNE 13-17, 1988) WILL HONOR PROFESSOR E. BRIGHT WILSON OF THE HARVARD UNIVERSITY ON THE OCCASION OF HIS 80TH BIRTHDAY.

WE ARE VERY GRATIFIED, INDEED, THAT THE NOBEL LAUREATE PROFESSOR KENNETH G. WILSON FROM CORNELL UNIVERSITY HAS ACCEPTED TO GIVE THE BANQUET LECTURE ON JUNE 15.

IT IS A TRIBUTE TO THIS CONFERENCE THAT THE WILSON FAMILY HAS ACCEPTED TO PARTICIPATE ACTIVELY. WHILE SOME ASPECTS OF PROFESSOR BRIGHT WILSON'S INTERESTS MAY RECEIVE PARTICULAR ATTENTION AT THE 1988 MEETINGS, WE DO ENCOURAGE CONTRIBUTIONS FROM ALL AREAS OF MOLECULAR SPECTROSCOPY. WE HOPE THAT YOU WILL COME TO THE 1988 SYMPOSIUM IN LARGE NUMBERS, PRESENT PAPERS AND HELP CELEBRATE THIS SPECIAL EVENT IN A GRAND MANNER.

Please see note on page 21 and respond

The invited speakers who have accepted so far are:

Nobel Laureates Dudley Herschbach (Harvard University)

and Yuan T. Lee (Univ. of California, Berkeley)

Drs. Jon T. Hougen (NBS, Washington, D.C.), James K. G.

Watson (Herzberg Institute of Astrophysics, Canada),

E. Hirota (Okazaki, Japan)

Drs. Manfred Winnewisser (Giessen, West Germany),

Gisbert Winnewisser (Köln, West Germany), H. W. Schrötter

(München, West Germany), Arlan Mantz (Spectra Physics-

Laser Analytics, Boston), H. Buijs (Bomem, Inc., Canada), n

and R. E. Smalley (Rice University, Texas)



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HIGH RESOLUTION FOURIER SPECTROSCOPY OF THE Ar⁺ LASER 5145 Å EXCITED I₂ FLUORESCENCE SPECTRUM

R. BACIS, S. CHURASSY, R. W. FIELD, J. B. KOFFEND, AND J. VERGES

This preliminary work demonstrates the feasibility of obtaining a high resolution spectrum of cw laser excited fluorescence using a Fourier spectrometer.

Using 1.3W of 5145 Å multimode power from an Ar⁺ laser, fluorescence is excited mainly via the P(13) and R(15) (43,0) lines. Nearly all of the fluorescence lines [P(13), P(17), R(11), R(15)] originating from v' = 43 are observed. Their recorded full width at half maximum in the 7000-8000 cm⁻¹ region is 0.85. rous odd-J" satellite lines. rotation-vibration levels of

Rotational relaxation (ΔJ' - The usual parameters are obtained I₂ X²Σ⁺ through v" = 85.

The vibrational line intensities are in agreement with the alternation pattern predicted by the Franck-Condon factors of Tellinghuisen. The agreement between measured and calculated intensities is only qualitative for high v" values. This has important implications with respect to the I₂ laser gain measurements discussed in the following talk.

¹J. Tellinghuisen, J. Quant. Spect. Rad. Transf. 19, 149 (1978).

Address of Bacis and Churassy: Laboratoire de Spectrométrie Ionique et Moléculaire 43, bd du 11 Novembre 1918, 69621 - Villeurbanne, France.

Address of Field and Koffend: Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139.

Address of Verges: Laboratoire Aimé Cotton - C.N.R.S. II, Bâtiment 505, 91405 - Orsay, France.

Time required: 15, 10 or 5 min.

* Session in which paper is recommended for presentation: _____

Chemical formulas & sketches of molecular structures for larger molecules:

- PLEASE NOTE:
1. Use good quality bond paper and an electric typewriter when preparing your Abstract. In the space for title and abstract you may include tables, equations and line drawings.
 2. Send an original and one copy.
 3. Please use a larger envelope for mailing. Do not fold.
 4. Underline the name of the person who will be presenting the paper.
 5. Include only the TITLE, AUTHORS' NAMES, and TEXT in the abstract. The author's affiliation should be given separately, as shown in the example.
 6. Supply chemical formulas and rough sketches of structures of the larger molecules. This information is useful in arranging sessions.

General categories of sessions:

- | | | |
|----------------------------------|---------------------|-------------------------------|
| (1) Electronic (large molecules) | (6) Laser spectra | (11) Raman spectra |
| (2) Electronic (small molecules) | (7) Liquid state | (12) Solid state (electronic) |
| (3) Electronic (theory) | (8) Matrix spectra | (13) Solid state (infrared) |
| (4) Energy transfer | (9) Microwave | (14) Techniques |
| (5) High resolution IR & THEORY | (10) Molecular beam | (15) Vibrational analysis |

PLEASE CHOOSE ONE OF THESE FIFTEEN CATEGORIES FOR YOUR PAPER AND GIVE THAT INFORMATION IN THE PLACE WHERE THE * APPEARS ABOVE. THANK YOU.

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MONDAY, JUNE 15, 1987 -- 8:45 A.M.

Auditorium, Independence Hall

Chairmen: JAMES C. GARLAND, Department of Physics, The Ohio State University, Columbus, Ohio.

R. S. McDOWELL, Los Alamos National Laboratory,
Los Alamos, New Mexico.

Plenary Session

Opening remarks by J. C. GARLAND.....8:45

MA1. FREQUENCY BASED SPECTROSCOPY FROM THE MICROWAVE TO THE VISIBLE.....40 min.

KENNETH EVENSON, Time and Frequency Division, National Bureau of Standards, Boulder, Colorado, 80303.

MA2. INFRARED MICROWAVE SIDEBAND LASER SPECTROSCOPY IN THE CO AND CO₂ LASER REGIONS.....40 min.

R. H. SCHWENDEMAN, Department of Chemistry, Michigan State University, East Lansing, Michigan, 48824-1322.

MA3. INTERPRETATION OF THE SPECTRA OF "AMMONIA-LIKE" MOLECULES-- FREQUENCIES AND INTENSITIES OF TRANSITIONS.....40 min.

S. URBAN, Czechoslovak Academy of Sciences, J. Hevrovský Institute of Physical Chemistry and Electrochemistry, 166 10 Prague 6, Czechoslovakia.

Intermission

COBLENTZ PRIZE AND AWARD LECTURE (11:15 A.M. - 12 Noon)

MA4. RAMAN SPECTROSCOPY OF MOLECULES ADSORBED ON SOLID SURFACES.....30 min.

A. CAMPION, Department of Chemistry, University of Texas, Austin, Texas, 78712.

PLEASE NOTE:

BOTH THE PLENARY SESSIONS ON MONDAY AND WEDNESDAY MORNINGS (JUNE 15 AND 17) WILL START AT 8:45 A.M.

MONDAY, JUNE 15, 1987 -- 1:30 P.M.

Room 2027, Robinson Laboratory

Chairman: PRABHAKAR MISRA, Department of Chemistry, The Ohio State University, Columbus, Ohio.

- ME1. INFRARED DETECTION OF HCOCNH^+ : OBSERVATION OF THE ν_1 (N-H STRETCH) FUNDAMENTAL BAND.....10 min.(1:30)

SANG K. LEE and T. AMANO, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.

- ME2. INFRARED SPECTROSCOPY OF NH^+ : AN ANALYSIS OF THE PERTURBATION BETWEEN THE $X^2\Pi$ AND $a^4\Sigma^-$ STATES.....15 min.(1:42)

K. KAWAGUCHI, Institute for Molecular Science, Okazaki, Japan; and T. AMANO, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.

- ME3. INFRARED SPECTRUM OF THE ν_3 BAND OF NH_2^+15 min.(1:59)

B. D. REHFUSS, M. OKUMURA, M. G. BAWENDI, T. OKA, Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois, 60637; and B. M. DINELLI, Istituto di Spettroscopia Molecolare del C.N.R., Bologna, Italy.

- ME4. INFRARED SPECTRUM OF THE ν_3 BAND OF NH_3^+15 min.(2:16)

M. G. BAWENDI, B. D. REHFUSS, M. OKUMURA, T. OKA, Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois, 60637; and B. M. DINELLI, Istituto di Spettroscopia Molecolare del C.N.R., Bologna, Italy.

- ME5. OBSERVATION OF SUB-DOPPLER INFRARED SPECTRUM OF THE H_3O^+ ION.....15 min.(2:33)

YIT-TSONG CHEN and TAKESHI OKA, Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois, 60637.

- ME6. DETERMINATION OF THE DIPOLE MOMENT OF ArH^+ FROM THE ROTATIONAL ZEEMAN EFFECT BY TUNABLE FAR INFRARED LASER SPECTROSCOPY.....15 min.(2:50)

K. LAUGHLIN, G. A. BLAKE, R. C. COHEN, D. C. HOVDE, and R. J. SAYKALLY, Department of Chemistry, University of California, Berkeley, California, 94720.

- ME7. THE RENNER TELLER EFFECT IN $X^2\Pi\text{CO}_2^+$10 min.(3:07)

J. M. FRYE and T. J. SEARS, Department of Chemistry, Brookhaven National Laboratory, Upton, New York, 11973.

Intermission

- ME8. VELOCITY MODULATION LASER SPECTROSCOPY OF NEGATIVE IONS: THE INFRARED SPECTRUM OF HYDROSULFIDE (SH^-).....10 min.(3:30)

M. GRUEBELE, M. POLAK, and R. J. SAYKALLY, Department of Chemistry, University of California, Berkeley, California, 94720.

- ME9. DIODE LASER VELOCITY MODULATION SPECTROSCOPY OF NEGATIVE IONS: THE ν_3 AND $\nu_3+\nu_2-\nu_2$ BANDS OF THIOCYANATE (NCS^-)..... 5 min.(3:42)

M. POLAK, M. GRUEBELE, and R. J. SAYKALLY, Department of Chemistry, University of California, Berkeley, California, 94720.

- ME10. VELOCITY MODULATION LASER SPECTROSCOPY OF NEGATIVE IONS: THE ν_3 BAND OF AZIDE (N_3^-)..... 5 min.(3:49)

M. POLAK, M. GRUEBELE, and R. J. SAYKALLY, Department of Chemistry, University of California, Berkeley, California, 94720.

- ME11. VELOCITY MODULATION INFRARED LASER SPECTROSCOPY OF NEGATIVE IONS:
THE ν_3 , $\nu_3+\nu_1-\nu_1$, $\nu_3+\nu_2-\nu_2$ AND $\nu_3+2\nu_2-2\nu_2$ BANDS OF CYANATE (NCO^-)..... 5 min. (3:56)
M. GRUEBELE, M. POLAK, and R. J. SAYKALLY, Department of
Chemistry, University of California, Berkeley, California, 94720.
- ME12. LABORATORY MEASUREMENTS OF THE ABUNDANCE RATIO $|\text{HCO}^+|/|\text{HOC}^+|$
AND THEIR ASTROPHYSICAL IMPLICATIONS.....15 min. (4:03)
T. AMANO, Herzberg Institute of Astrophysics, National Research
Council of Canada, Ottawa, Ontario, Canada, K1A 0R6; and
T. NAKANAGA, National Laboratory for Chemical Industry, Tsukuba,
Japan.
- ME13. OBSERVATION OF THE ν_1 AND ν_3 FUNDAMENTAL BANDS OF H_2Cl^+15 min. (4:20)
SANG K. LEE, T. AMANO, Herzberg Institute of Astrophysics, National
Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6;
M. OLDANI, Laboratorium fur Physikalische Chemie, Eidgenossische
Technische Hochschule Zurich, CH-8092 Zurich, Switzerland; and
K. KAWAGUCHI, Institute for Molecular Science, Okazaki 444, Japan.
- ME14. THE ν_1 AND ν_3 FUNDAMENTAL BANDS OF SH_3^+15 min. (4:37)
T. NAKANAGA, National Laboratory for Chemical Industry, Tsukuba,
Japan; and T. AMANO, Herzberg Institute of Astrophysics,
National Research Council of Canada, Ottawa, Ontario, Canada,
K1A 0R6.
- ME15. INITIAL ASSIGNMENT OF THE PROTONATED ACETYLENE VIBRATION-ROTATION
SPECTRUM.....15 min. (4:54)
M. W. CROFTON, Lawrence Livermore National Laboratory, Livermore,
California, 95440; M.-F. JAGOD, B. D. REHFUSS, and T. OKA,
Department of Chemistry and Department of Astronomy and Astro-
Physics, The University of Chicago, Chicago, Illinois, 60637.
- ME16. INFRARED SPECTRUM OF THE ν_3 BAND OF C_2H_2^+15 min. (5:11)
M.-F. JAGOD, B. D. REHFUSS, T. OKA, Department of Chemistry and
Department of Astronomy and Astrophysics, The University of
Chicago, Chicago, Illinois, 60637; and M. W. CROFTON, Lawrence
Livermore National Laboratory, Livermore, California, 95440.

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MONDAY, JUNE 15, 1987 -- 1:30 P.M.

Room 1009, Physics Laboratory

Chairman Before Intermission: D. S. PERRY, Department of Chemistry,
The University of Akron, Akron, Ohio.

Chairman After Intermission: W. E. BLASS, Department of Physics and
Astronomy, University of Tennessee, Knoxville,
Tennessee.

MF1. THE VIBRATIONAL AND ROTATIONAL SPECTRA OF OZONE FOR THE
(0,1,0) AND (0,2,0) STATES.....15 min.(1:30)

H. M. PICKETT, E. A. COHEN, L. R. BROWN, Jet Propulsion Laboratory,
California Institute of Technology, Pasadena, California, 91109;
C. P. RINSLAND, M.A.H. SMITH, Atmospheric Sciences Division, MS 401A,
NASA Langley Research Center, Hampton, Virginia, 23665-2552;
V. MALATHY DEVI, Department of Physics, College of William and
Mary, Williamsburg, Virginia, 23185; A. GOLDMAN, Department of
Physics, University of Denver, Denver, Colorado, 80208;
A. BARBE, Laboratoire de Spectrométrie Moléculaire et Atmosphérique,
CNRS, Faculté des Sciences, Reims 51062, France; B. CARLI,
Istituto di Ricerca sulle Onde Elettromagnetiche CNR-IROE,
Firenze, Italy; and M. CARLOTTI, Istituto di Chimica Fisica
e Spettroscopia, Università di Bologna, 40136 Bologna, Italy.

MF2. INTENSITIES AND ANALYSIS OF THE $\nu_1 + \nu_2$ AND $\nu_2 + \nu_3$ BANDS OF $^{16}\text{O}_3$
NEAR 5.7 μm10 min.(1:47)

V. MALATHY DEVI, Department of Physics, College of William and
Mary, Williamsburg, Virginia, 23185; J.-M. FLAUD, C. CAMY-PEYRET,
Laboratoire de Physique Moléculaire et Atmosphérique, Université
Pierre et Marie Curie, CNRS, 75252 Paris, France; C. P. RINSLAND,
and M.A.H. SMITH, Atmospheric Sciences Division, MS 401A, NASA
Langley Research Center, Hampton, Virginia, 23665-5225;

MF3. PRESSURE-INDUCED LINE SHIFTS AND WIDTHS OF O_3 BROADENED BY N_2 AND BY AIR....10 min.(1:59)

M.A.H. SMITH, C. P. RINSLAND, Atmospheric Sciences Division,
MS 401A, NASA Langley Research Center, Hampton, Virginia,
23665-5225; V. MALATHY DEVI, and D. CHRIS BENNER, Department of
Physics, College of William and Mary, Williamsburg, Virginia,
23185.

MF4. THE PURE ROTATIONAL SPECTRUM OF $^{14}\text{N}^{16}\text{O}_2$10 min.(2:11)

A. PERRIN, J.-M. FLAUD, C. CAMY-PEYRET, Laboratoire de Physique
Moléculaire et Atmosphérique, Université Pierre et Marie Curie,
75252 Paris, France; B. CARLI, Istituto di Ricerca sulle Onde
Elettromagnetiche CNR-IROE, 50127 Firenze, Italy; and
M. CARLOTTI, Istituto di Chimica Fisica e Spettroscopia,
Università di Bologna, 40136 Bologna, Italy.

MF5. ANALYSIS OF THE 3 μm BANDS OF BENZENE.....15 min.(2:23)

J. PLIVA, Department of Physics, The Pennsylvania State University,
University Park, Pennsylvania, 16802; and A. S. PINE, Molecular
Spectroscopy Division, National Bureau of Standards, Gaithersburg,
Maryland, 20899.

MF6. HIGH RESOLUTION FOURIER TRANSFORM SPECTRUM OF DISULFANE, H_2S_2 ,
BETWEEN 30 AND 90 cm^{-1}15 min.(2:40)

G. M. PLUMMER, G. WINNEWISSER, I. Physikalisches Institut,
Universität zu Köln, 500 Köln 41, Federal Republic of Germany;
B. P. WINNEWISSER, and M. WINNEWISSER, Physikalisches-Chemisches
Institut, Justus-Liebig-Universität Giessen, 6300 Giessen,
Federal Republic of Germany.

Intermission

- MF7. EXTENSIVE VIBRATIONAL STATE MIXING OF INDIVIDUAL ROTATIONAL LEVELS IN 1-BUTYNE NEAR 3333 CM^{-1} 15 min.(3:10)
A. M. DE SOUZA, DEVINDER KAUR, and D. S. PERRY, Department of Chemistry, The University of Akron, Akron, Ohio, 44325.
- MF8. ASSIGNMENT OF CH₃OH FIR LASER LINES FROM NON-CO-STRETCH STATES.....15 min.(3:27)
I. MUKHOPADHYAY, M. MOLLABASHI, R. M. LEES, Department of Physics, University of New Brunswick, Fredericton, New Brunswick, Canada, E3B 5A3; W. LEWIS-BEVAN, Department of Chemistry, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Y6; and J.W.C. JOHNS, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.
- MF9. LASER STARK SPECTRA OF $^{13}\text{CH}_3\text{OH}$ AT 311 μm AND 337 μm10 min.(3:44)
G. R. SUDHAKARAN, L. H. JOHNSTON, J. SARKER, and R. BHATTACHARJEE, Department of Physics, University of Idaho, Moscow, Idaho, 83843.
- MF10. ON THE ASSIGNMENT OF THE HIGH EFFICIENCY 127 μm FIR LASER LINE OF $^{13}\text{CD}_3\text{OH}$ AND OTHER CH₃OH, CD₃OH AND CD₃OD FIR LASER LINES.....15 min.(3:56)
I. MUKHOPADHYAY, M. MOLLABASHI, R. M. LEES, Department of Physics, University of New Brunswick, Fredericton, New Brunswick, Canada, E3B 5A3; and W. LEWIS-BEVAN, Department of Chemistry, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Y6.
- MF11. LASER STARK SPECTROSCOPY OF CD₃OD at 337 μm WITH THE HCN LASER.....15 min.(4:13)
J. C. SARKER, L. H. JOHNSTON, G. R. SUDHAKARAN, R. L. BHATTACHARJEE, Department of Physics, University of Idaho, Moscow, Idaho, 83843.
- MF12. FREE JET INFRARED ABSORPTION SPECTROSCOPY OF THE ν_6 AND ν_7 BANDS OF IRON PENTACARBONYL.....15 min.(4:30)
YOSHIYASU MATSUMOTO, TETSURO MAJIMA, and MICHIO TAKAMI, The Institute of Physical and Chemical Research, Wako, Saitama 351-01, Japan.
- MF13. INFRARED BAND STRENGTH MEASUREMENTS OF CF₂.....10 min.(4:47)
J. WORMHOUDT, Center for Chemical and Environmental Physics, Aerodyne Research, 45 Manning Road, Billerica, Massachusetts, 01821.
- MF14. OBSERVATION AND ANALYSIS OF THE XeF₂ 1030 CM^{-1} BANDS..... 5 min.(4:59)
RICHARD W. SCHWENZ, Department of Chemistry, University of Northern Colorado, Greeley, Colorado, 80639; and D. J. DONALDSON, Department of Chemistry and Biochemistry, University of Colorado, Boulder, Colorado, 80309.

MONDAY, JUNE 15, 1987 -- 1:30 P.M.

Room 1005, Physics Laboratory

Chairman Before Intermission: L. JOHNSTON, Department of Physics, University of Idaho, Moscow, Idaho.

Chairman After Intermission: S. G. KUKOLICH, Department of Chemistry, The University of Arizona, Tucson, Arizona.

MG1. MICROWAVE SPECTRUM AND STRUCTURE OF CYCLOBUTENE OZONIDE AND CYCLOBUTADIENE OZONIDE.....10 min.(1:30)

P. LORENCAK, H. BADAWI, D. BORSETH, K. W. HILLIG, II, R. L. KUCZKOWSKI, Department of Chemistry, University of Michigan, Ann Arbor, Michigan, 48109; and G. D. MENDENHALL, Department of Chemistry and Chemical Engineering, Michigan Technological University, Houghton, Michigan, 49931.

MG2. MILLIMETER WAVE SPECTRUM OF THE PRIMARY OZONIDE OF ETHYLENE.....15 min.(1:42)

J. ZOZOM, C. W. GILLIES, Department of Chemistry, Rensselaer Polytechnic Institute, Troy, New York, 12180; R. D. SUENRAM, and F. J. LOVAS, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899.

MG3. ROTATIONAL SPECTRA OF ¹³C TAGGED PROPYNE IN THE V₁₀ VIBRATION.....10 min.(1:59)

J. A. ROBERTS, I. AN, and H. TAM, Department of Physics, North Texas State University, Denton, Texas, 76203.

MG4. MICROWAVE SPECTRUM OF BIS-TRIFLUOROMETHYL NITROXIDE.....15 min.(2:11)

R. M. WHITE, Department of Chemistry, College of Saint Benedict, St. Joseph, Minnesota, 56374; and J. D. GRAYBEAL, Department of Chemistry, Virginia Tech, Blacksburg, Virginia, 24061.

MG5. THE MICROWAVE SPECTRA, QUADRUPOLE COUPLING CONSTANTS, AND STRUCTURE OF N-CHLORODIFLUOROMETHANIMINE AND N-BROMODIFLUOROMETHANIMINE.....15 min.(2:28)

P. GRONER, H. NAWAIE, J. R. DURIG, Department of Chemistry, University of South Carolina, Columbia, South Carolina, 29208; and D. DES MARTEAU, Department of Chemistry, Clemson University, Clemson, South Carolina, 29631.

MG6. MICROWAVE SPECTRUM AND STRUCTURE OF THE SO₂ - H₂S COMPLEX.....15 min.(2:45)

R. E. BUMGARNER, D. J. PAULEY, and S. G. KUKOLICH, Department of Chemistry, The University of Arizona, Tucson, Arizona, 85721.

Intermission

MG7. THE ROTATIONAL SPECTRUM, STRUCTURE AND DIPOLE MOMENT OF ETHYNYLPHOSPHINE, H₂PC≡CH.....10 min.(3:15)

E. A. COHEN, G. A. McRAE, S. DI STEFANO, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California, 91109; R. A. BEAUDET, Department of Chemistry, Center for the Study of Fast Transient Processes, University of Southern California, Los Angeles, California, 90089-0482; and H. GOLDWHITE, Department of Chemistry, California State University Los Angeles, Los Angeles, California, 90032.

MG8. MICROWAVE SPECTRUM OF METHYL DIFLUOROPHOSPHATE.....15 min.(3:27)

L. RICKUS, H. JUSTINES, J. ZOZOM, C. W. GILLIES, Department of Chemistry, Rensselaer Polytechnic Institute, Troy, New York, 12180; F. J. LOVAS, R. D. SUENRAM, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899; and T. DIGIUSEPPE, Geo-Center, Inc., Seven Wells Avenue, Newton Center, Massachusetts, 02159.

- MG9. THE MICROWAVE SPECTRUM OF ARGON-PHOSPHORUS TRIFLUORIDE.....10 min. (3:44)
K. W. HILLIG, II, J. MATOS, A. SCIOLY, and R. L. KUCZKOWSKI,
Department of Chemistry, University of Michigan, Ann Arbor,
Michigan, 48109.
- MG10. HIGH RESOLUTION ROTATIONAL SPECTROSCOPY OF A WEAKLY BOUND IONIC CLUSTER:
Ar.H₃⁺ AND DEUTERATED ISOTOPOMERS.....15 min. (3:56)
M. BOGEY, H. BOLVIN, C. DEMUYNCK, and J. L. DESTOMBES, Laboratoire
de Spectroscopie Hertzienne, Associé au CNRS, Université de Lille I,
F 59655 Villeneuve d'Ascq, France.
- MG11. MICROWAVE SPECTRA OF NOBLE GAS-PYRIDINE COMPLEXES.....15 min. (4:13)
T. D. KLOTS, T. EMILSSON, R. S. RUOFF, C. CHUANG, and H. S. GUTOWSKY,
Noyes Chemical Laboratory, University of Illinois, Urbana, Illinois,
61801.
- MG12. TUNNELING IN DIBORANE-HYDROGEN CHLORIDE DIMERS.....15 min. (4:30)
CARL CHUANG, T. D. KLOTS, R. S. RUOFF, T. EMILSSON, and H. S. GUTOWSKY,
Noyes Chemical Laboratory, University of Illinois, Urbana, Illinois,
61801.
- MG13. EXPERIMENTAL SEPARATION OF TORSIONAL AND CHARGE REDISTRIBUTION EFFECTS
IN ROTATIONAL SPECTRA OF HCN DIMERS.....15 min. (4:47)
R. S. RUOFF, T. EMILSSON, C. CHUANG, T. D. KLOTS, and H. S. GUTOWSKY,
Noyes Chemical Laboratory, University of Illinois, Urbana, Illinois,
61801.
- MG14. FTMW STUDIES OF HYDROGEN-BONDED TRIMERS.....15 min. (5:04)
R. S. RUOFF, T. D. KLOTS, C. CHUANG, T. EMILSSON, and H. S. GUTOWSKY,
Noyes Chemical Laboratory, University of Illinois, Urbana, Illinois,
61801.

MONDAY, JUNE 15, 1987 -- 1:30 P.M.

Room 214, Denney Hall

CHAIRMAN: C. J. WURREY, Department of Chemistry, University of Missouri-Kansas City, Kansas City, Missouri.

MH1. OPTICAL CONSTANTS OF C_4N_2 - AN APPLICATION TO TITAN'S ATMOSPHERE.....10 min.(1:30)

M. A. PERERA-JARMER and R. K. KHANNA, Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland, 20742.

MH2. ABSOLUTE INTENSITIES AND COMPLEX REFRACTIVE INDICES OF CRYSTALLINE HC_3N IN THE INFRARED REGION.....10 min.(1:42)

C. M. HUDSON and R. K. KHANNA, Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland, 20742.

MH3. DIFFERENTIAL REFLECTION SPECTROSCOPY: A DIRECT DETERMINATION OF LONG WAVELENGTH OPTICAL MODE FREQUENCIES IN POLAR CRYSTALS.....10 min.(1:54)

M. E. THOMAS and R. I. JOSEPH, Applied Physics Laboratory, The Johns Hopkins University, Laurel, Maryland, 20707.

MH4. INFRARED SPECTROSCOPY OF CO ADSORBED ON SODIUM CHLORIDE SURFACES.....15 min.(2:06)

H. H. RICHARDSON and G. E. EWING, Department of Chemistry, Indiana University, Bloomington, Indiana, 47405.

MH5. CRYSTAL VIBRATION OF BETA BARIUM METABORATE AND ITS PHASE TRANSITION BY RAMAN SCATTERING.....15 min.(2:23)

GUOZHEN WU, BOGANG TIAN, and XAOJUN LAI, Laboratory of Vibrational Spectroscopy, Institute of Chemistry, Academia Sinica, Beijing, China.

MONDAY, JUNE 15, 1987 -- 3:00 P.M.

Room 214, Denney Hall

CHAIRMAN: C. J. WURREY, Department of Chemistry, University of Missouri-Kansas City, Kansas City, Missouri.

- MH'1. TRANSFER AND STORAGE OF VIBRATIONAL ENERGY IN LIQUIDS: COLLISIONAL UP-PUMPING OF CARBON MONOXIDE ON LIQUID ARGON.....15 min.(3:00)
R. DISSELKAMP and G. E. EWING, Department of Chemistry, Indiana University, Bloomington, Indiana, 47405.
- MH'2. TIME-RESOLVED FLUORESCENCE DEPOLARIZATION OF DODCI IN ETHYLENE GLYCOL: EFFECT OF ORIENTATIONAL CORRELATION ON ELECTRONIC EXCITATION TRANSPORT.....10 min.(3:17)
P. A. AFINRUD and W. S. STRUVE, Department of Chemistry and Ames Laboratory-USDOE, Iowa State University, Ames, Iowa, 50011.
- MH'3. INTERNAL ROTATION-VIBRATION COUPLING CONTRIBUTIONS TO VIBRATIONAL LEVEL MIXING IN S_1 p-FLUORTOLUENE.....15 min.(3:29)
R. J. LONGFELLOW and C. S. PARMENTER, Department of Chemistry, Indiana University, Bloomington, Indiana, 47405.
- MH'4. DETERMINATION OF THE TORSIONAL POTENTIAL IN GLYOXAL BY ELECTRONIC SPECTROSCOPY.....15 min.(3:46)
K. W. BUTZ, J. J. JOHNSON, D. J. KRAJNOVICH, and C. S. PARMENTER, Department of Chemistry, Indiana University, Bloomington, Indiana, 47405.
- MH'5. THE p-DIFLUOROBENZENE-AR VAN DER WAALS COMPLEX. SPECTROSCOPY, IVR AND VIBRATIONAL PREDISSOCIATION.....15 min.(4:03)
K. W. BUTZ, H.-K. O, M.-C. SU, and C. S. PARMENTER, Department of Chemistry, Indiana University, Bloomington, Indiana, 47405.
- MH'6. VIBRATIONALLY INELASTIC SCATTERING FROM I_2 AND GLYOXAL IN A NEW CROSSED MOLECULAR BEAM EXPERIMENT.....15 min.(4:20)
K. W. BUTZ, DU HONG, D. KRAJNOVICH, and C. S. PARMENTER, Department of Chemistry, Indiana University, Bloomington, Indiana, 47405.
- MH'7. ROTATIONAL AND VIBRATIONAL COLLISIONAL ENERGY TRANSFER IN $^{13}CH_3F$15 min.(4:37)
H. EVERITT, F. C. DE LUCIA, Department of Physics, Duke University, Durham, North Carolina, 27706; R. I. McCORMICK, Department of Physics, United States Military Academy, West Point, New York, 10996; and D. D. SKATRUD, Physics Division, Army Research Office, Research Triangle Park, North Carolina, 27709.
- MH'8. $CN B^2\Sigma^+$ ALIGNMENT FOLLOWING VUV DISSOCIATION OF ICN.....15 min.(4:54)
J. A. GUEST, Department of Chemistry, University of Cincinnati, Cincinnati, Ohio, 45221; and F. WEBSTER, Department of Chemistry and the James Franck Institute, University of Chicago, Chicago, Illinois, 60637.
- MH'9. PHOTOFRAGMENTATION SPECTROSCOPY OF ALKYL NITRITES IN THE $\pi-\pi^*$ CHARGE TRANSFER BAND.....15 min.(5:11)
SALLY S. HUNNICUTT, Department of Chemistry, University of Cincinnati, Cincinnati, Ohio, 45221; and CHARLES A. WIGHT, Department of Chemistry, University of Utah, Salt Lake City, Utah, 84112.

TUESDAY, JUNE 16, 1987 -- 8:30 A.M.

Room 2027, Robinson Laboratory

Chairman: R. E. MILLER, Department of Chemistry, University of North Carolina, Chapel Hill, North Carolina.

TA1. DEUTERIUM NUCLEAR HYPERFINE SPLITTINGS OF ROTATIONAL TRANSITIONS.....15 min. (8:30)

S. JANS-BÜRLI and A. BAUDER, Laboratorium für Physikalische Chemie, Eidgenössische Technische Hochschule, CH-8092 Zürich, Switzerland.

TA2. ISOTOPE EFFECTS IN THE HIGH RESOLUTION INFRARED SPECTRA OF OC-HF.....10 min. (8:47)

G. T. FRASER and A. S. PINE, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899.

TA3. ROTATIONAL SPECTRUM AND STRUCTURE OF $H_2CO-HCl$15 min. (8:59)

C. W. GILLIES, J. ZOZOM, Department of Chemistry, Rensselaer Polytechnic Institute, Troy, New York, 12181; G. T. FRASER, F. J. LOVAS, and R. D. SUENRAM, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899.

TA4. ROTATIONAL SPECTRA OF $Ar-CH_3OH$, $Ar-CD_3OH$, AND $Kr-CH_3OH$15 min. (9:16)

R. D. SUENRAM, G. T. FRASER, F. J. LOVAS, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899; J. ZOZOM, and C. W. GILLIES, Department of Chemistry, Rensselaer Polytechnic Institute, Troy, New York, 12181.

TA5. ROTATIONAL SPECTRUM AND INTERNAL ROTATION IN CH_3OH-NH_315 min. (9:33)

G. T. FRASER, F. J. LOVAS, and R. D. SUENRAM, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899.

TA6. VIBRATIONAL PREDISSOCIATION SPECTROSCOPY OF HCN CLUSTERS.....15 min. (9:50)

D. S. ANEX and G. E. EWING, Department of Chemistry, Indiana University, Bloomington, Indiana, 47405.

Intermission

TA7. NEGATIVE ION PHOTOELECTRON SPECTROSCOPY OF $Rb_{n=2,3}^-$15 min. (10:20)

K. M. MCHUGH, J. G. EATON, G. H. LEE, K. H. BOWEN, Department of Chemistry, The Johns Hopkins University, Baltimore, Maryland, 21218; and J. S. SNODGRASS, Department of Chemistry, University of California-Santa Barbara, Santa Barbara, California, 93106.

TA8. NEGATIVE ION PHOTOELECTRON SPECTROSCOPY OF: $NO^-(Ar)_1$, $NO^-(Kr)_1$, $NO^-(Xe)_1$, AND N_2O_215 min. (10:37)

C. B. FREIDHOFF, Westinghouse R & D Center, Pittsburgh, Pennsylvania; G. H. LEE, J. T. SNODGRASS, and K. H. BOWEN, Department of Chemistry, The Johns Hopkins University, Baltimore, Maryland, 21218.

TA9. VIBRATIONAL PREDISSOCIATION SPECTROSCOPY OF CLUSTER IONS: INFRARED SPECTRA OF THE CLUSTERS H_n^+ AND $H_3O^+(H_2)_m$15 min. (10:54)

M. OKUMURA, Department of Chemistry, The University of Chicago, Chicago, Illinois, 60637; L. I. YEH, and Y. T. LEE, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, and Department of Chemistry, University of California, Berkeley, California, 94720.

- TA10. INFRARED SPECTRA OF THE HYDRATED HYDRONIUM ION CLUSTERS $H_3O^+ \cdot (H_2O)_m$,
 $m=1-3$15 min. (11:11)
M. OKUMURA, Department of Chemistry, The University of Chicago,
Chicago, Illinois, 60637; L. I. YEH, J. D. MYERS, and Y. T. LEE,
Materials and Molecular Research Division, Lawrence Berkeley
Laboratory, and Department of Chemistry, University of California,
Berkeley, California, 94720.
- TA11. SOLVATED ALKALI ION CLUSTERS: PRODUCTION AND PRELIMINARY VIBRATIONAL
PREDISSOCIATION SPECTRA.....15 min. (11:28)
WEN-LONG LIU and JAMES M. LISY, Department of Chemistry, University
of Illinois at Urbana-Champaign, Urbana, Illinois, 61801.
- TA12. AN INVESTIGATION OF THE "SOFT" TORSIONAL MODES OF $(HF)_3$15 min. (11:45)
KIRK D. KOLENBRANDER and JAMES M. LISY, School of Chemical Sciences,
University of Illinois at Urbana-Champaign, Urbana, Illinois, 61801.
- TA13. HIGH VIBRATIONAL LEVEL SPECTROSCOPY OF POTASSIUM DIMER.....10 min. (12:02)
JOHN S. OZCOMERT and PATRICK L. JONES, Department of Chemistry,
The Ohio State University, Columbus, Ohio, 43210.

TUESDAY, JUNE 16, 1987 — 8:30 A.M.

Room 1009, Physics Laboratory

Chairman: D. CHRIS BENNER, Department of Physics, College of William and Mary, Williamsburg, Virginia.

- TB1. THE RELATIVE MERITS OF POLARIZING VS AMPLITUDE DIVISION FOURIER TRANSFORM SPECTROSCOPY.....15 min. (8:30)
H. BULJS and C. TRIPP, Bomem Inc., 625 Rue Marais, Vanier, Quebec, Canada, G1M 2Y2.
- TB2. EXPERIMENTAL RESULTS FROM THE LOS ALAMOS FOURIER TRANSFORM SPECTROMETER.....15 min. (8:47)
B. PALMER and R. S. McDOWELL, Los Alamos National Laboratory, University of California, Los Alamos, New Mexico, 87545.
- TB3. LINESHIFT MODULATION FOURIER TRANSFORM SPECTROSCOPY.....15 min. (9:04)
M. ELHANINE, R. FARRENG, and G. GUELACHVILI, Laboratoire d'Infrarouge, Associé au CNRS, Université Paris XI, 91405 Orsay, France.
- TB4. FUNDAMENTAL LIMITS TO PRECISION IN MEASUREMENT OF PEAK HEIGHT, POSITION, AND WIDTH IN FOURIER TRANSFORM SPECTROSCOPY.....10 min. (9:21)
A. G. MARSHALL and L. CHEN, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.
- TB5. NEW HETERODYNE FREQUENCY MEASUREMENTS ON OCS AND FREQUENCY CALIBRATION TABLES BASED ON OCS AND N₂O.....15 min. (9:33)
A. G. MAKI, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899; and J. S. WELLS, Time and Frequency Division, National Bureau of Standards, Boulder, Colorado, 80303.
- TB6. USING A WAVEMETER WITH TUNABLE INFRARED DIODE LASERS.....15 min. (9:50)
M. D. MARSHALL, H. LEW, N. MARMET, A.R.W. McKELLAR, and G. W. NICHOLS, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.
- TB7. NEAR-INFRARED SPECTROSCOPY WITH DFB LASERS.....15 min. (10:07)
H. SASADA, Department of Physics, Faculty of Science and Technology, Keio University, 14-1 Hiyoshi 3-Chome, Kohoku-ku, Yokohama, 223 Japan.
- Intermission
- TB8. QUADRATIC HERMAN-WALLIS FACTORS FOR THE FUNDAMENTALS OF LINEAR MOLECULES....15 min. (10:35)
JAMES K.G. WATSON, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.
- TB9. ABSOLUTE INTENSITY MEASUREMENTS OF THE 2.7 μm BANDS OF CO₂.....10 min. (10:52)
C. M. DEELEY and J.W.C. JOHNS, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.
- TB10. ABSOLUTE INTENSITY MEASUREMENTS IN THE ν_2 AND ν_3 FUNDAMENTALS OF CO₂.....15 min. (11:04)
J.W.C. JOHNS, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.
- TB11. TDL INVESTIGATION OF THE Q-BRANCH OF CO₂ NEAR 720 cm^{-1}10 min. (11:21)
T. HUET, N. LACOME, and A. LEVY, Laboratoire d'Infrarouge, Associé au CNRS, Université Paris-Sud, 91405 Orsay, France.

- TB12. ν_2 REGION OF CO_2 : TEMPERATURE DEPENDENCE OF N_2 - AND SELF-BROADENING COEFFICIENTS.....15 min.(11:33)
- T. HUET, G. GUELACHVILI, N. LACOME, A. LEVY, Laboratoire d'Infrarouge, Université de Paris-Sud, 91405 Orsay, France; C. CHACKERIAN, NASA-Ames Research Center, Moffett Field, California, 94035; and K. NARAHARI RAO, Department of Physics, The Ohio State University, Columbus, Ohio, 43210.
- TB13. COLLISIONAL LINE MIXING IN AN N_2 -BROADENED CO_2 Q BRANCH.....10 min.(11:50)
- L. L. STROW, Department of Physics, University of Maryland Baltimore County, Catonsville, Maryland, 21228; and B. M. GENTRY, Code 617, NASA/Goddard Space Flight Center, Greenbelt, Maryland, 20771.
- TB14. COLLISIONAL LINE MIXING IN N_2O Q BRANCHES.....10 min.(12:00)
- L. L. STROW, Department of Physics, University of Maryland Baltimore County, Catonsville, Maryland, 21228; and A. S. PINE, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899.
- TB15. FB13 will be presented here (Mark P. Esplin).....5 min.(12:12)

TUESDAY, JUNE 16, 1987 -- 8:30 A.M.

Room 1005, Physics Laboratory

Chairman Before Intermission: J. M. GINDER, Department of Physics, The Ohio State University, Columbus, Ohio.

Chairman After Intermission: JONATHAN E. KENNY, Department of Chemistry, Tufts University, Medford, Massachusetts.

TC1. ABSOLUTE FLUORESCENCE QUANTUM YIELDS OF AZULENE FROM THE S_1 MANIFOLD.....15 min. (8:30)

SUDHIR K. KULKARNI and JONATHAN E. KENNY, Department of Chemistry, Tufts University, Medford, Massachusetts, 02155.

TC2. HYDROGEN BONDING IN GROUND AND EXCITED STATES OF PYRAZINE.....15 min. (8:47)

TE-YANG LIU, JONATHAN E. KENNY, Department of Chemistry, Tufts University, Medford, Massachusetts, 02155; and WILLIAM R. MOOMAW, Department of Chemistry, Williams College, Williamstown, Massachusetts, 02167.

TC3. FLUORESCENCE QUANTUM YIELDS OF JET-COOLED AZULENES.....15 min. (9:04)

TIMOTHY M. WOODENBERG, Perkin-Elmer Corp., 761 Main Avenue, Norwalk, Connecticut, 06859; SUDHIR K. KULKARNI, and JONATHAN E. KENNY, Department of Chemistry, Tufts University, Medford, Massachusetts, 02155.

TC4. STRUCTURE DEPENDENT COMPETITION BETWEEN MULTIPHOTON ABSORPTION AND INTRAMOLECULAR ENERGY REDISTRIBUTION IN ORGANOMOLYBDENUM COMPOUNDS: STATE SELECTIVE PRODUCTION OF MOLYBDENUM ATOMS.....15 min. (9:21)

BRIAN SAMORISKI and J. CHAIKEN, Department of Chemistry, Syracuse University, Syracuse, New York, 13244-1200.

TC5. GAS PHASE ELECTRONIC SPECTROSCOPY OF ARENE CHROMIUM TRICARBONYLS: DIRECT DISSOCIATION VS. PREDISSOCIATION IN THE LOWEST ENERGY EXCITED ELECTRONIC STATE.....15 min. (9:38)

DAN ROONEY and J. CHAIKEN, Department of Chemistry, Syracuse University, Syracuse, New York, 13244-1200.

TC6. ELECTRONIC TRANSITION MOMENT DIRECTIONS OF THE ADENINE CHROMOPHORE.....10 min. (9:55)

LEIGH B. CLARK, Department of Chemistry, University of California-San Diego, La Jolla, California, 92093.

Intermission

TC7. HYDROGEN BONDED CLUSTERS OF TRYPTOPHAN AND RELATED COMPOUNDS.....15 min. (10:25)

L. A. PETEANU, L. A. PHILIPS, Y. D. PARK, and D. H. LEVY, James Franck Institute, University of Chicago, Chicago, Illinois, 60637.

TC8. SPECTROSCOPY OF JET-COOLED p-DICHLOROBENZENE AND p-DICHLOROBENZENE - ARGON VAN DER WAALS COMPLEX.....15 min. (10:42)

W. D. SANDS and R. MOORE, Department of Chemistry, Virginia Commonwealth University, Richmond, Virginia, 23284.

TC9. CHEMILUMINESCENCE FROM LASER-HEATED SOLID AND GASEOUS TETRAMETHYLDIOXETANE.....15 min. (10:59)

M. A. TOLBERT, M. J. ROSSI, and D. L. HUESTIS, Chemical Physics Laboratory, SRI International, Menlo Park, California, 94025.

TC10. PHOTOINDUCED ABSORPTION IN EMERALDINE.....15 min.(11:16)

J. M. GINDER, M. G. ROE, P. E. WIGEN, Department of Physics,
The Ohio State University, Columbus, Ohio, 43210; A. J. EPSTEIN,
Department of Physics and Department of Chemistry, The Ohio
State University, Columbus, Ohio, 43210; M. ANGELOPOULOS, and
A. G. MACDIARMID, Department of Chemistry, University of
Pennsylvania, Philadelphia, Pennsylvania, 19104.

TC11. INTRACONFIGURATIONAL ABSORPTION AND VISIBLE REGION ABSORPTION SPECTROSCOPY
OF ReCl_6^{2-} IN VARIOUS $(\text{NR}_4)_2\text{SnCl}_6$ HOST CRYSTALS.....10 min.(11:33)

S. C. LEE, R. K. YOO, T. A. KEIDERLING, Department of Chemistry,
University of Illinois at Chicago, Chicago, Illinois, 60680; and
B. A. KOZIKOWSKI, Procter and Gamble, Miami Valley Laboratories,
Cincinnati, Ohio, 45247.

TC12. ELECTRONIC SPECTROSCOPY AND ENERGY TRANSFER PATHWAYS FOR MATRIX
ISOLATED I_2Arrived Late.....15 min.(11:45)

WAFAA FAWZY, M.A.P. MACLER, M. C. HEAVEN, Department of Chemistry,
Emory University, Atlanta, Georgia, 30322; and J. P. NICOLAI,
Department of Chemical Engineering, Massachusetts Institute of
Technology, Cambridge, Massachusetts, 02139.

TUESDAY, JUNE 16, 1987 -- 8:30 A.M.

Room 214, Denney Hall

Chairman: V. F. KALASINSKY, Department of Chemistry, Mississippi State University, Mississippi State, Mississippi.

- TD1. FTIR ISOTOPIC STUDY OF THE C_2H_3 VINYL RADICAL IN AN ARGON MATRIX.....15 min. (8:30)
RICHARD A. SHEPHERD and W.R.M. GRAHAM, Department of Physics, Texas Christian University, Fort Worth, Texas, 76129.
- TD2. VIBRATIONAL AND ELECTRONIC SPECTRA OF THE PRODUCTS OF THE H + HCN REACTION TRAPPED IN SOLID ARGON.....15 min. (8:47)
MARILYN E. JACOX, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899.
- TD3. INFRARED SPECTRA OF GUEST MOLECULES IN CRYSTALLINE CLATHRATE HYDRATE FILMS.....15 min. (9:04)
J. PAUL DEVLIN and FOUAD FLEYFEL, Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma, 74074.
- TD4. THE USE OF ISOLATED ISOTOPOMER SPECTRA IN PROBING THE DEFECT STRUCTURE OF ICE.....15 min. (9:21)
PAUL J. WOOLDRIDGE and J. PAUL DEVLIN, Department of Chemistry, Oklahoma State University, Stillwater, Oklahoma, 74074.
- TD5. Ag₇ CLUSTER: PENTAGONAL BIPYRAMID.....15 min. (9:38)
S.B.H. FACH, R. J. VAN ZEE, W. WELTNER, JR., Department of Chemistry, University of Florida, Gainesville, Florida, 32611; and D. G. GARLAND, City University of New York, The City College, New York, New York, 10031.
- TD6. GROUND STATE OF THE C₆ MOLECULE.....15 min. (9:55)
R. J. VAN ZEE, W. WELTNER, JR., Department of Chemistry, University of Florida, Gainesville, Florida, 32611; R. F. FERRANTE, Department of Chemistry, Wake Forest University, Winston-Salem, North Carolina, 27109; and K. J. ZERINGUE, Nicols Research Corporation, Huntsville, Alabama.
- Intermission
- TD7. C_nO MOLECULES.....10 min. (10:25)
R. J. VAN ZEE and W. WELTNER, JR., Department of Chemistry, University of Florida, Gainesville, Florida, 32611.
- TD8. THE SEARCH FOR PYRIDYNE: MATRIX ISOLATION OF 2,3- AND 3,4-PYRIDINEDICARBOXYLIC ANHYDRIDE AND THEIR PHOTOLYSIS PRODUCTS.....15 min. (10:37)
H.-H. NAM and G. E. LEROI, Department of Chemistry, Michigan State University, East Lansing, Michigan, 48824.
- TD9. MATRIX ISOLATION SPECTROSCOPY FOR VIBRATIONAL ASSIGNMENTS AND GROUP FREQUENCY DETERMINATIONS.....15 min. (10:54)
D. PRESSER, Mattson Instruments, Inc., 1001 Fourier Court, Madison, Wisconsin, 53717; and R. J. JAKOBSEN, Mattson Institute for Spectroscopic Research, The Ohio State University Research Park, 1224 Kinnear Road, Columbus, Ohio, 43212.
- TD10. OPTICAL AND ESR SPECTROSCOPY OF MATRIX-ISOLATED ETHYLNITRENE.....15 min. (11:11)
ROBERT F. FERRANTE, SUSAN L. ERICKSON, Department of Chemistry, Wake Forest University, Winston-Salem, North Carolina, 27109; and BRIAN M. PEEK, Department of Chemistry, University of North Carolina-Chapel Hill, Chapel Hill, North Carolina, 27514.

TD11. MAGNETIC CIRCULAR DICHROISM OF CYCLOOCTATETRAFYNYL MONOANIONS ISOLATED IN
ARGON MATRICES..... Arrived Late.....15 min. (11:28)

C. SAMET, J. LURITO, L. ANDREWS and P. N. SCHATZ, Department of
Chemistry, University of Virginia, Charlottesville, Virginia,
22901.

TUESDAY, JUNE 16, 1987 -- 1:30 P.M.

Room 2027, Robinson Laboratory

SEMINAR ON PROBING AND MODELING THE EARTH'S ATMOSPHERE

CHAIRMAN: LAURENCE S. ROTHMAN, Optics Division, Air Force Geophysics
Laboratory, Hanscom Air Force Base, Massachusetts.

INVITED PAPERS

- TE1. IMPLICATIONS OF THE ATMOS(ATMOSPHERIC TRACE MOLECULE SPECTROSCOPY)
EXPERIMENT.....30 min.(1:30)

LINDA R. BROWN, Jet Propulsion Laboratory, California Institute
of Technology, Pasadena, California, 91109.

- TE2. HIGH RESOLUTION INFRARED MEASUREMENTS AT TEMPERATURES RELEVANT TO
ATMOSPHERIC PROBING.....30 min.(2:03)

PRASAD VARANASI, Laboratory for Planetary Atmospheres Research,
State University of New York at Stony Brook, Stony Brook,
New York, 11794-2300.

- TE3. HIGH RESOLUTION INFRARED SPECTROSCOPY AS A PROBE OF THE MIDDLE
ATMOSPHERE.....30 min.(2:36)

J.-M. FLAUD and C. CAMY-PEYRET, Laboratoire de Physique Moléculaire
et D'Optique Atmosphérique, C.N.R.S., Campus D'Orsay, 91405 Orsay,
France.

Intermission

- TE4. THE SCRIBE INTERFEROMETER SYSTEM AND EMISSION MEASUREMENTS OF THE
EARTH'S ATMOSPHERE.....30 min.(3:20)

GEORGE A. VANASSE, Infrared Physics Branch, Optical Physics Division,
Air Force Geophysics Laboratory, Hanscom Air Force Base,
Massachusetts, 01731-5000.

- TE5. MEASUREMENTS AND ANALYSIS OF THE STRATOSPHERIC FAR-INFRARED EMISSION
SPECTRUM.....30 min.(3:53)

BRUNO CARLI, Istituto di Ricerca Sulle Onde Elettromagnetiche,
Consiglio Nazionale delle Ricerche, 50127 Firenze, Italy.

CONTRIBUTED PAPERS

- TE6. GAS CORRELATION SPECTROSCOPY OF THE STRATOSPHERE: THE HALOGEN
OCULTATION EXPERIMENT (HALOE).....10 min.(4:26)

D. CHRIS BENNER, Department of Physics, College of William and Mary,
Williamsburg, Virginia, 23185; S. ROLAND DRAYSON, Department of
Atmospheric and Oceanic Science, University of Michigan, Ann Arbor,
Michigan, 48109; and JAMES M. RUSSELL III, Atmospheric Sciences
Division, MS 401B, NASA Langley Research Center, Hampton,
Virginia, 23665-5225.

- TE7. STRATOSPHERIC NO_x GAS DISTRIBUTIONS FROM BALLOON-BORNE THERMAL EMISSION
SPECTRA.....10 min.(4:38)

W. A. SHAFFER, L. W. HERATH, Science Systems and Applications, Inc.,
Seabrook, Maryland, 20706; M. M. ABBAS, Department of Physics and
Atmospheric Sciences, Drexel University, Philadelphia, Pennsylvania,
19104; J. C. BRASUNAS, V. G. KUNDE, W. C. MAGUIRE, Code 693.2,
Goddard Space Flight Center, Greenbelt, Maryland, 20771; A. GOLDMAN,
Department of Physics, University of Denver, Denver, Colorado,
80208; J. R. HERMAN, Code 610.0, Goddard Space Flight Center,
Greenbelt, Maryland, 20771; and S. T. MASSIE, National Center for
Atmospheric Research, P.O. Box 3000, Boulder, Colorado, 80307.

TE8. LOWER STRATOSPHERIC TRACE CONSTITUENTS FROM A BALLOON-BORNE
CRYOGENIC INTERFEROMETER.....10 min. (4:50)

W. C. MAGUIRE, J. C. BRASUNAS, V. G. KUNDE, Code 693.2, Goddard Space Flight Center, Greenbelt, Maryland, 20771; M. M. ABBAS, Department of Physics and Atmospheric Sciences, Drexel University, Philadelphia, Pennsylvania, 19104; A. GOLDMAN, Department of Physics, University of Denver, Denver, Colorado, 80208; L. W. HERATH, W. A. SHAFFER, Science Systems and Applications, Inc., Seabrook, Maryland, 20706; J. R. HERMAN, Code 610.0, Goddard Space Flight Center, Greenbelt, Maryland, 20771; and S. T. MASSIE, National Center for Atmospheric Research, P. O. Box 3000, Boulder, Colorado, 80307.

TUESDAY, JUNE 16, 1987 -- 1:30 P.M.

Room 1009, Physics Laboratory

Chairman: BRADLEY M. STONE, Department of Chemistry, San Jose State University, San Jose, California.

- TF1. FORBIDDEN ROTATION TRANSITIONS BETWEEN NUCLEAR SPIN MODIFICATIONS IN POLYATOMIC MOLECULES BY NUCLEAR SPIN-ROTATION INTERACTIONS.....15 min. (1:30)

MAN-CHOR CHAN, TAKESHI OKA, Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois, 60637; and K. LALITA SARKAR, Department of Physics, Indian Institute of Technology, Kanpur-16, India.

- TF2. THE ANOMALOUS $k=3$ SPLITTINGS OF PH_3 IN THE v_2 STATE OBSERVED BY RADIOFREQUENCY-INFRARED DOUBLE-RESONANCE.....15 min. (1:47)

YIT-TSONG CHEN and TAKESHI OKA, Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois, 60637.

- TF3. OBSERVATION OF SMALL SPLITTINGS IN THE VIBRATION-ROTATION SPECTRUM OF PF_515 min. (2:04)

JOHN ERVE, YIT-TSONG CHEN, and TAKESHI OKA, Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois, 60637.

- TF4. INFRARED MICROWAVE SIDEBAND LASER SPECTROSCOPY IN THE CO LASER REGION.....15 min. (2:21)

SHIN-CHU HSU, R. H. SCHWENDEMAN, Department of Chemistry, Michigan State University, East Lansing, Michigan, 48824; and GOTTFRIED MAGERL, Institut für Nachrichtentechnik und Hochfrequenztechnik, Technical University of Vienna, A-1040 Vienna, Austria.

- TF5. INFRARED MICROWAVE DOUBLE RESONANCE WITH A SIDEBAND LASER SPECTROMETER.....15 min. (2:38)

DEAN B. PETERSON and R. H. SCHWENDEMAN, Department of Chemistry, Michigan State University, East Lansing, Michigan, 48824.

- TF6. EXPERIMENTAL DETERMINATION OF ELECTRIC FIELDS IN THE POSITIVE COLUMN OF A GLOW DISCHARGE..... 5 min. (2:55)

M. B. RADUNSKY and R. J. SAYKALLY, Department of Chemistry, University of California, Berkeley, California, 94720.

Intermission

- TF7. EFFICIENCY AND LINewidth IMPROVEMENTS IN A GRAZING INCIDENCE DYE LASER USING AN INTRACAVITY LENS AND SPHERICAL END MIRROR.....10 min. (3:20)

R. S. SMITH and L. F. DIMAURO, Department of Physics, Louisiana State University, Baton Rouge, Louisiana, 70803.

- TF8. DIODE LASER SPECTROSCOPY OF $a^3\Pi$ (∞)... (WITHDRAWN).....10 min. (3:32)

P. B. DAVIES and P. A. MARTIN, Department of Physical Chemistry, University of Cambridge, Cambridge CB2 1EP, England.

- TF9. LASER INDUCED FLUORESCENCE OF CO^+ AND THE $CO a^3\Pi_1$ STATE PRODUCED BY 2+1 MULTIPHOTON ABSORPTION IN A SUPERSONIC JET.....10 min. (3:44)

M. ANSELMONT, L. F. DIMAURO, Department of Physics, Louisiana State University, Baton Rouge, Louisiana, 70803; and T. A. MILLER, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

- TF10. INFRARED SPECTRUM OF THE FO_2 RADICAL.....15 min. (3:56)

A.R.W. MCKELLAR, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6; J. B. BURKHOLDER, A. SINHA, and C. J. HOWARD, NOAA Aeronomy Laboratory, R/E/AL2, 325 Broadway, Boulder, Colorado, 80303, and Department of Chemistry and Biochemistry and CIRES, University of Colorado, Boulder, Colorado, 80309.

- TF11. DIODE LASER SPECTROSCOPY OF THE ν_2 BAND OF THE CD_3 RADICAL.....10 min.(4:13)
J. M. FRYE and T. J. SEARS, Department of Chemistry, Brookhaven
National Laboratory, Upton, New York, 11973.
- TF12. NEW VIBRATIONAL BANDS FROM THE $\Pi(010)$ STATE OF THE CCH RADICAL IN THE
GROUND ELECTRONIC STATE.....10 min.(4:25)
H. KANAMORI and E. HIROTA, Institute for Molecular Science,
Okazaki 444, Japan.
- TF13. Π_{12} will be presented here (LESLIE M. TACK).....10 min.(4:37)
- TF14. Π_{14} will be presented here (A. FAIBIS).....10 min.(4:49)
- TF15. Π_{15} will be presented here (AUREL FAIBIS).....10 min.(5:01)

A RESPONSE IS REQUESTED:

IN CONNECTION WITH THE ANNOUNCEMENT AT THE BEGINNING OF THIS BOOKLET IT WOULD HELP IF YOU CAN INFORM ME BY A NOTE AT THE REGISTRATION DESK ABOUT YOUR ANTICIPATIONS FOR COMING TO THE 1988 BANQUET. WE WILL EXPLORE OTHER VENUES SHOULD THE NUMBERS GO OVER THE LIMIT OF WHAT THE FACULTY CLUB CAN ACCOMMODATE. I REALIZE THAT IT MAY SEEM PREMATURE TO BE THINKING OF 1988 AT THIS POINT IN TIME, BUT YOU WILL UNDERSTAND THAT RESERVATIONS FOR FACILITIES HAVE TO BE MADE FAR IN ADVANCE.

THANK YOU.

RAO

MAY 7, 1987

TUESDAY, JUNE 16, 1987 -- 1:30 P.M.

Room 1005, Physics Laboratory

Chairman Before Intermission: S. P. REDDY, Department of Physics, Memorial University of Newfoundland, St. John's, Newfoundland, Canada.

Chairman After Intermission: P. F. BERNATH, Department of Chemistry, University of Arizona, Tucson, Arizona.

TG1. HIGH RESOLUTION FOURIER TRANSFORM EMISSION SPECTROSCOPY OF XeH.....15 min. (1:30)

M. DOUAY, S. A. ROGERS, and P. F. BERNATH, Department of Chemistry, University of Arizona, Tucson, Arizona, 85721.

TG2. HIGH RESOLUTION VIBRATION-ROTATION EMISSION SPECTRA OF XeH⁺ AND CH.....15 min. (1:47)

S. A. ROGERS, C. R. BRAZIER, and P. F. BERNATH, Department of Chemistry, University of Arizona, Tucson, Arizona, 85721.

TG3. THE ELECTRONIC STRUCTURE OF GAS PHASE MnH.....15 min. (2:04)

T. D. VARBERG, J. A. GRAY, and R. W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139.

TG4. A NEW SPUTTER SOURCE AND ITS APPLICATION TO THE NiH SPECTRUM.....15 min. (2:21)

MINGGUANG LI, J. A. GRAY, and R. W. FIELD, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139.

TG5. THE GREEN BANDS OF CaO: OODR SPECTROSCOPY AND ELECTRONIC STRUCTURE MODEL...15 min. (2:38)

DAVID P. BALDWIN, R. W. FIELD, and J. NORMAN, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139.

TG6. THE LOW LYING STATES OF SAMARIUM OXIDE.....15 min. (2:55)

C. LINTON, GUO BUJIN, Department of Physics, University of New Brunswick, Fredericton, New Brunswick, Canada, E3B 5A3; R. S. RANA, Department of Physics, Holy Cross College, Worcester, Massachusetts, 01610; and J. A. GRAY, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139.

Intermission

TG7. VIBRATIONAL ASSIGNMENT FOR THE A²Π-X²Σ BAND SYSTEM OF THE SiN RADICAL: THE 0-0 BAND OF ²⁹SiN AND ³⁰SiN.....15 min. (3:25)

CHIKASHI YAMADA, EIZI HIROTA, Institute for Molecular Science, Okazaki, 444 Japan; SATOSHI YAMAMOTO, and SHUJI SAITO, Nagoya University, Nagoya, 460 Japan.

TG8. HIGH RESOLUTION LASER SPECTROSCOPY OF NIOBIUM NITRIDE.....15 min. (3:42)

Y. AZUMA, J. A. BARRY, M.J.P. LYNE, A. J. MERER, Department of Chemistry, University of British Columbia, Vancouver, British Columbia, Canada, V6T 1Y6; and J. O. SCHRÖDER, Institut für Molekülphysik, Freie Universität Berlin, D-1000 Berlin 33, Germany.

TG9. THE FIRST NEGATIVE BAND SYSTEM OF ¹⁵N₂⁺15 min. (3:59)

S. PADDI REDDY and C.V.V. PRASAD, Department of Physics, Memorial University of Newfoundland, St. John's, Newfoundland, Canada, A1B 3X7.

- TG10. ABSOLUTE ABSORPTION CROSS SECTION MEASUREMENTS OF OZONE AND THE TEMPERATURE DEPENDENCE.....10 min. (4:16)
K. YOSHINO, D. E. FREEMAN, and W. H. PARKINSON, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, 02138.
- TG11. UPPER STATE OF THE SCHUMANN-RUNGE BANDS OF OXYGEN: TRIPLET FINE STRUCTURES FOR $^{16}\text{O}^{18}\text{O}$ AND $^{18}\text{O}_2$10 min. (4:28)
A.S.-C. CHEUNG, Department of Chemistry, University of Hong Kong, Hong Kong; K. YOSHINO, D. E. FREEMAN, and W. H. PARKINSON, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, 02138.
- TG12. PREDISSOCIATION LINE WIDTHS OF THE SCHUMANN-RUNGE BANDS OF $^{16}\text{O}_2$10 min. (4:40)
A.S.-C. CHEUNG, Department of Chemistry, University of Hong Kong, Hong Kong; K. YOSHINO, D. E. FREEMAN, J. R. ESMOND, and W. H. PARKINSON, Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts, 02138.
- TG13. A HIGH RESOLUTION STUDY OF THE VACUUM ULTRAVIOLET ABSORPTION SPECTRUM OF CS.....10 min. (4:52)
G. STARK, K. YOSHINO, and P. L. SMITH, Harvard-Smithsonian Center For Astrophysics, Cambridge, Massachusetts, 02138.

TUESDAY, JUNE 16, 1987 -- 1:30 P.M.

Room 214, Denney Hall

Chairman: RUSSELL BARNES, Battelle Columbus Laboratories,
Columbus, Ohio.

TH1. VIBRATIONAL ANALYSIS OF PENTAHALIDE METAL COMPLEXES.....15 min. (1:30)

E. M. NOUR, Department of Chemistry, Qatar University, Doha 2713,
Qatar (Arabian Gulph).

TH2. INFRARED AND RAMAN SPECTRA OF GASEOUS, LIQUID, AND SOLID METHYL AND
METHYL-d₃ VINYL SULFIDE AND THE CONFORMATIONAL STABILITY IN THE GAS PHASE...15 min. (1:47)

T. J. DICKSON and J. R. DURIG, Department of Chemistry,
University of South Carolina, Columbia, South Carolina, 29208.

TH3. COMPUTATION OF VIBRATIONAL SPECTRA OF N-ALKANES.....15 min. (2:04)

B. GALABOV, T. DUDEV, Department of Chemistry, University of
Sofia, Sofia 1126, Bulgaria; and J. R. DURIG, Department of
Chemistry, University of South Carolina, Columbia, South
Carolina, 29208.

TH4. INFRARED AND RAMAN SPECTRA, CONFORMATIONAL STABILITY AND VIBRATIONAL
ASSIGNMENT OF CYCLOBUTYLGERMANE.....15 min. (2:21)

T. J. GEYER, T. S. LITTLE, J. R. DURIG, Department of Chemistry,
University of South Carolina Columbia, South Carolina, 29208;
and M. DAKKOURI, Abteilung für Physikalische Chemie, Universität
Ulm, 7900 Ulm, West Germany.

TH5. RAMAN AND FAR INFRARED SPECTRA, CONFORMATIONAL STABILITIES, AND
BARRIERS TO INTERNAL ROTATION OF SEVERAL PERFLUOROMETHYL ALCOHOLS.....15 min. (2:38)

R. A. LARSEN, F. O. COX, J. R. DURIG, Department of Chemistry,
University of South Carolina, Columbia, South Carolina, 29208;
and B. J. VAN DER VEKEN, Laboratorium voor Anorganische
Scheikunde, Rijksuniversitair Centrum Antwerpen, B2020 Antwerpen,
Belgium.

TH6. INFRARED AND RAMAN SPECTRA, VIBRATIONAL ASSIGNMENT, NORMAL COORDINATE
ANALYSIS, AND BARRIER TO INTERNAL ROTATION OF N-CHLORO-N-METHYL
METHANAMINE.....15 min. (2:55)

N. E. LINDSAY, J. R. DURIG, Department of Chemistry, University of
South Carolina, Columbia, South Carolina, 29208; and T. J. HIZER,
Department of Natural Sciences, Claflin College, Orangeburg,
South Carolina, 29115.

Intermission

TH7. ON THE VIBRATIONAL SPECTRUM OF METHYL NITRITE.....10 min. (3:25)

HOWARD D. STIDHAM, Department of Chemistry, University of
Massachusetts, Amherst, Massachusetts, 01003; G. A. GUIRGIS,
and J. R. DURIG, Department of Chemistry, University of
South Carolina, Columbia, South Carolina, 29208.

TH8. VIBRATIONAL SPECTRA AND CONFORMATIONS OF (CHLOROMETHYL)THIIRANE.....15 min. (3:37)

C. J. WURREY, Y.-Y. CHIEN, F. G. ROJAS, P. M. GREEN, Department
of Chemistry, University of Missouri, Kansas City, Missouri,
64110; and V. F. KALASINSKY, Department of Chemistry,
Mississippi State University, Mississippi State, Mississippi, 39762.

TH9. INFRARED SPECTRA OF THE HALOGEN ISOCYANATE AND THIOCYANATE
VAPOR MOLECULES.....15 min. (3:54)

T. C. DEVORE, Department of Chemistry, James Madison University,
Harrisonburg, Virginia, 22807.

TH10. VIBRATIONAL SPECTRA OF TRANS-1,2-DIFLUOROETHYLENE OXIDE.....10 min.(4:11)

N. C. CRAIG, K. S. PRANATA, Department of Chemistry, Oberlin College, Oberlin, Ohio, 44074; and C. W. GILLIES, Department of Chemistry, Rensselaer Polytechnic Institute, Troy, New York, 12180.

TH11. MINDO CALCULATIONS AND VIBRATIONAL DYNAMICS OF DL- β -BUTYROLACTONE.....15 min.(4:23)

P. VANEERDEN and D. McDERMOTT, Department of Chemistry, Lafayette College, Easton, Pennsylvania, 18042.

TH12. VIBRATIONAL SPECTRA, CONFORMATIONS, AND BARRIERS TO INTERNAL ROTATION IN CYCLOHEXYLSILANE AND PROPYLSILANE.....15 min.(4:40)

R. C. KENTON, S. SUBRAMANIAM, and V. F. KALASINSKY, Department of Chemistry, Mississippi State University, Mississippi State, Mississippi, 39762.

TH13. VIBRATIONAL FREQUENCIES FOR POLYATOMIC MOLECULES.....15 min.(4:57)

WILLIAM B. COLLIER, National Institute for Petroleum and Energy Research, P.O. Box 2128, Bartlesville, Oklahoma, 74005.

WEDNESDAY, JUNE 17, 1987 -- 8:45 A.M.

Auditorium, Independence Hall

Chairmen: K. NARAHARI RAO, Department of Physics, The Ohio State University, Columbus, Ohio.

A.R.W. MCKELLAR, Herzberg Institute of Astrophysics,
The National Research Council, Ottawa, Ontario, Canada.

WA1. THE SPECTROSCOPY OF WEAK BONDS.....40 min.

WILLIAM KLEMPERER, Department of Chemistry, Harvard University, Cambridge, Massachusetts, 02138.

WA2. INFRARED SPECTROSCOPY OF WEAKLY BOUND MOLECULAR COMPLEXES FORMED IN NOZZLE EXPANSIONS.....40 min.

B. J. HOWARD, Physical Chemistry Laboratory, Oxford University, Oxford OX1 3QZ, England.

Intermission

WA3. ROTATIONAL STUDIES OF VAN DER WAALS COMPLEXES COMPRISED OF ASYMMETRIC TOP SUBUNITS.....40 min.

FRANK LOVAS, Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland, 20899.

WA4. QUANTUM AND CLASSICAL INTERACTIONS AFFECTING THE SPECTRA OF WEAKLY BOUND COMPLEXES.....40 min.

CLIFFORD E. DYKSTRA, School of Chemical Sciences, University of Illinois at Urbana-Champaign, Urbana, Illinois, 61801.

WEDNESDAY, JUNE 17, 1987 -- 1:30 P.M.

Room 2027, Robinson Laboratory

Chairman Before Intermission: C. W. GILLIES, Department of Chemistry,
Rensselaer Polytechnic Institute, Troy, New York.

Chairman After Intermission: A. BAUDER, Laboratorium für Physikalische Chemie,
Eidgenössische Technische Hochschule, Zurich,
Switzerland.

WE1. ROTATIONAL SPECTRA OF s-trans AND s-cis GLYOXAL-d₁ (CHO-CDO)
OBSERVED BY MICROWAVE FOURIER TRANSFORM SPECTROSCOPY.....15 min. (1:30)

M. RÖDLER, M. OLDANI, and A. BAUDEK, Laboratorium für Physikalische
Chemie, Eidgenössische Technische Hochschule, CH-8092 Zurich,
Switzerland.

WE2. MILLIMETER WAVE SPECTRA OF METHYL-AND DEUTERATED-CYANOACETYLENE,
CH₃C₃N AND DC₃N, IN SOME EXCITED VIBRATIONAL STATES.....15 min. (1:47)

K.M.T. YAMADA, G. M. PLUMMER, M. BESTER, G. WINNEWISSER,
I. Physikalisches Institut, Universität zu Köln, 5000 Köln 41,
Federal Republic of Germany; M. TANIMOTO, Sagami Chemical
Research Center, Nish-Ohnuma, Sagamihara, Kanagawa 229, Japan;
and K. MÖLLER, Physikalisches-Chemisches Institut, Justin-Liebig
Universität Giessen, 6300 Giessen, Federal Republic of Germany.

WE3. THE WATER DIMER: THEORY AND MEASUREMENTS.....15 min. (2:04)

L. H. COUDERT, J. T. HOUGEN, F. J. LOVAS, and R. D. SUENRAM,
Molecular Spectroscopy Division, National Bureau of Standards,
Gaithersburg, Maryland, 20899.

WE4. GLOBAL FIT OF ROTATIONAL ENERGY LEVELS OF THE GROUND VIBRATIONAL STATE
OF METHYLAMINE OBTAINED FROM MICROWAVE, FAR-INFRARED PURE ROTATIONAL,
AND FAR-INFRARED TORSIONAL BAND TRANSITIONS.....15 min. (2:21)

N. OHASHI, Department of Physics, Faculty of Science, Kanazawa
University, Kanazawa 920, Japan; K. TAKAGI, Department of Physics,
Faculty of Science, Toyama University, Toyama 930, Japan;
W. J. LAFFERTY, W. B. OLSON, and J. T. HOUGEN, Molecular
Spectroscopy Division, National Bureau of Standards, Gaithersburg,
Maryland, 20899.

WE5. CALCULATION OF THE TORSIONAL-ROTATIONAL ENERGY LEVELS OF CH₂DXH AND
CHD₂XH.....15 min. (2:38)

MUJIAN LIU and C. RICHARD QUADE, Department of Physics, Texas
Tech University, Lubbock, Texas, 79409.

WE6. ROTATIONAL SPECTROSCOPY OF THE EXCITED VIBRATIONAL STATES OF HNO₃.....15 min. (2:55)

R. L. CROWNOVER, F. C. DE LUCIA, Department of Physics, Duke
University, Durham, North Carolina, 27706; R. A. BOOKER,
Department of Physics, University of North Carolina at Ashville,
Ashville, North Carolina, 28804; and P. HELMINGER, Department
of Physics, University of South Alabama, Mobile, Alabama, 36688.

Intermission

WE7. MILLIMETER AND SUBMILLIMETER SPECTROSCOPY OF SMALL INTERNAL ROTORS.....15 min. (3:25)

T. ANDERSON, R. L. CROWNOVER, S. L. SHOSTAK, E. HERBST, and
F. C. DE LUCIA, Department of Physics, Duke University,
Durham, North Carolina, 27706.

WE8. SUBMILLIMETER LASER STARK SPECTROSCOPY SYSTEM.....10 min. (3:42)

L. JOHNSTON, G. SUDHAKARAN, J. SARKER, R. BHATTACHARJEE, Department
of Physics, University of Idaho, Moscow, Idaho, 83843; R. SRIVISTAVA,
Department of Computer Science, University of Waterloo, Waterloo,
Ontario, Canada, N2L 3G1; S. RAJU, Hughes Aircraft Co., P.O. Box
92919, S/C Building 541, MS B326, Los Angeles, California, 90009;
and D. HASEROT, P.O. Box 8729, Moscow, Idaho, 83843.

WE9. GAS PHASE SPECTROSCOPY IN A COLLISIONALLY COOLED CELL NEAR 4K.....15 min.(3:54)

D. WILLEY, R. L. CROWNOVER, and F. C. DE LUCIA, Department of Physics,
Duke University, Durham, North Carolina, 27706.

WE10. MICROWAVE SPECTROSCOPY OF THE ELECTRONICALLY EXCITED STATES
($a^3\Pi_r$ AND $a^3\Sigma^+$) OF CO.....15 min.(4:11)

SATOSHI YAMAMOTO and SHUJI SAITO, Department of Astrophysics,
Nagoya University, Chikusa-ku, Nagoya 464, Japan.

WE11. DETECTION AND EQUILIBRIUM MOLECULAR STRUCTURE OF A SHORT-LIVED
MOLECULE, HBO, BY INFRARED DIODE LASER AND MICROWAVE SPECTROSCOPY.....15 min.(4:28)

Y. KAWASHIMA, Ikutoku Technical University, 1030 Shimo-ogino,
Atsugi, Kanagawa 243-02, Japan; K. KAWAGUCHI, Y. ENDO,
and E. HIROTA, Institute for Molecular Science, Okazaki 444,
Japan.

WE12. THE MICROWAVE SPECTRUM OF THE PH_2 RADICAL..... 5 min.(4:45)

MASATOSHI KAJITA, YASUKI ENDO, and EIZI HIROTA, Institute for
Molecular Science, Myodaiji, Okazaki 444, Japan.

WE13. THE MILLIMETER AND SUBMILLIMETER WAVE SPECTRA OF PROTONATED AND
DEUTERATED NITROUS OXIDE.....10 min.(4:52)

M. BOGEY, C. DEMUYNCK, J. L. DESTOMBES, Laboratoire de
Spectroscopie Hertzienne, Associé au CNRS, Université de Lille I,
F-59655 Villeneuve d'Ascq, France; and A.R.W. MCKELLAR,
Herzberg Institute of Astrophysics, National Research Council
of Canada, Ottawa, Ontario, Canada, K1A 0R6.

WEDNESDAY, JUNE 17, 1987 -- 1:30 P.M.

Room 1009, Physics Laboratory

Chairman Before Intermission: JOEL MULLINGHUISEN, Department of Chemistry,
Vanderbilt University, Nashville, Tennessee.

Chairman After Intermission: J. L. HARDWICK, Chemical Physics Institute,
University of Oregon, Eugene, Oregon.

WF1. STUDY OF THE ELECTRONIC GROUND STATE OF NH_2 BY LASER EXCITED FLUORESCENCE
FOURIER TRANSFORM SPECTROSCOPY.....15 min.(1:30)

M. VERVLOET, Herzberg Institute of Astrophysics, National Research
Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.

WF2. EMISSION BANDS OF THE $\tilde{A}^2A' - \tilde{X}^2A''$ SYSTEM OF HO_215 min.(1:47)

E. H. FINK, H. KRUSE, Physikalisches Chemie-Fachbereich 9, Bergische
Universität-Gesamthochschule Wuppertal, D-5600 Wuppertal 1,
Federal Republic of Germany; and D. A. RAMSAY, Herzberg Institute
of Astrophysics, National Research Council of Canada, Ottawa,
Ontario, Canada, K1A 0R6.

WF3. NEW INFRARED OBSERVATIONS OF THE H_3 MOLECULE.....15 min.(2:04)

W. A. MAJEWSKI, Department of Chemistry, University of Pittsburgh,
Pittsburgh, Pennsylvania, 15260; and J.K.G. WATSON, Herzberg
Institute of Astrophysics, National Research Council of Canada,
Ottawa, Ontario, Canada, K1A 0R6.

WF4. ROTATIONALLY COLD EMISSION IN THE $A^2\Pi_1 - X^2\Pi_r$ SYSTEM OF SO^+15 min.(2:21)

I. W. MILKMAN, J. C. CHOI, J. L. HARDWICK, and J. T. MOSELEY,
Chemical Physics Institute, University of Oregon, Eugene,
Oregon, 97403-1274.

WF5. FORMATION OF O^- IONS IN THE MULTIPHOTON EXCITATION OF NO15 min.(2:38)

Y. ONO, J. L. HARDWICK, and J. T. MOSELEY, Chemical Physics
Institute, University of Oregon, Eugene, Oregon, 97403-1274.

WF6. INFRARED SPECTROSCOPY OF THE $A^2\Pi_u + X^2\Sigma_g^+$ (0,1) HOT BAND OF C_2^- USING
TUNABLE DIODE LASER SPECTROMETER.....15 min.(2:55)

DI-JIA LIU, WING-CHEUNG HO, and TAKESHI OKA, Department of Chemistry
and Department of Astronomy and Astrophysics, The University of
Chicago, Chicago, Illinois, 60637.

WF7. FOURIER TRANSFORM SPECTROSCOPY OF THE $A^2A - X^2\Pi$ ELECTRONIC TRANSITION OF THE
JET COOLED CCl FREE RADICAL.....10 min.(3:12)

L. C. O'BRIEN, C. R. BRAZIER, and P. F. BERNATH, Department of
Chemistry, University of Arizona, Tucson, Arizona, 85721.

Intermission

WF8. HIGH RESOLUTION LASER SPECTROSCOPY OF CALCIUM ACETYLIDE (CaCCH).....15 min.(3:35)

A.M.R.P. BOPEGEDERA, C. R. BRAZIER, and P. F. BERNATH, Department
of Chemistry, University of Arizona, Tucson, Arizona, 85721.

WF9. HIGH RESOLUTION LASER SPECTROSCOPY OF CaCH_3 AND SrCH_315 min.(3:52)

C. R. BRAZIER and P. F. BERNATH, Department of Chemistry,
University of Arizona, Tucson, Arizona, 85721.

WF10. HIGH RESOLUTION LASER SPECTROSCOPY OF STRONTIUM MONOCYANATE, SrNCO10 min.(4:09)

L. C. O'BRIEN and P. F. BERNATH, Department of Chemistry,
University of Arizona, Tucson, Arizona, 85721.

WF11. HIGH RESOLUTION LASER SPECTROSCOPY OF CaN_3 AND SrN_315 min.(4:21)

C. R. BRAZIER and P. F. BERNATH, Department of Chemistry,
University of Arizona, Tucson, Arizona, 85721.

WF12 and WF13 will be presented here (W. KETTERLE).....25 min.(4:38)

WEDNESDAY, JUNE 17, 1987 -- 1:30 P.M.

Room 1005, Physics Laboratory

Chairman Before Intermission: WILLIS B. PERSON, Department of Chemistry,
University of Florida, Gainesville, Florida.

Chairman After Intermission: R. W. LOVEJOY, Department of Chemistry,
Lehigh University, Bethlehem, Pennsylvania.

WG1. HIGH RESOLUTION FOURIER TRANSFORM SPECTROSCOPY OF ACETYLENE: THE
BENDING REGION.....15 min.(1:30)

J. J. HILLMAN, D. E. JENNINGS, Laboratory for Extraterrestrial
Physics, NASA/Goddard Space Flight Center, Greenbelt, Maryland,
20771; G. W. HALSEY, Center for Drilling and Well Technology,
Rogaland Research Institute, P.O. Box 2503, Ullandhaug,
40001 Stavanger, Norway; and W. E. BLASS, Molecular
Spectroscopy Laboratory, Department of Physics and Astronomy,
The University of Tennessee, Knoxville, Tennessee, 37996-1200.

WG2. THE ν_3 SPECTRAL REGION OF CS_2 : SPECTRA.....10 min.(1:47)

V. MALATHY DEVI, D. CHRIS BENNER, Department of Physics,
College of William and Mary, Williamsburg, Virginia, 23185;
GUY GUELACHVILI, Laboratoire d'Infrarouge, Université de
Paris-Sud, Associé au CNRS, Orsay, France; and K. NARAHARI RAO,
Department of Physics, The Ohio State University, Columbus,
Ohio, 43210.

WG3. THE ν_3 SPECTRAL REGION OF CS_2 : ASSIGNMENTS AND MOLECULAR CONSTANTS.....10 min.(1:59)

D. CHRIS BENNER, V. MALATHY DEVI, Department of Physics,
College of William and Mary, Williamsburg, Virginia, 23185;
GUY GUELACHVILI, Laboratoire d'Infrarouge, Université de
Paris-Sud, Associé au CNRS, Orsay, France; and K. NARAHARI RAO,
Department of Physics, The Ohio State University, Columbus,
Ohio, 43210.

WG4. AIR-BROADENED AND NITROGEN-BROADENED WIDTH COEFFICIENTS AND PRESSURE
SHIFTS IN THE ν_4 AND ν_2 BANDS OF $^{12}CH_4$10 min.(2:11)

C. P. RINSLAND, M.A.H. SMITH, Atmospheric Sciences Division,
Mail Stop 401A, NASA Langley Research Center, Hampton, Virginia,
23665-5225; V. MALATHY DEVI, and D. CHRIS BENNER, Department of
Physics, College of William and Mary, Williamsburg, Virginia, 23185.

WG5. AIR-BROADENED LORENTZ HALFWIDTHS IN THE ν_4 BAND OF $^{13}CH_4$ USING A
FOURIER TRANSFORM SPECTROMETER.....10 min.(2:23)

V. MALATHY DEVI, D. CHRIS BENNER, Department of Physics,
College of William and Mary, Williamsburg, Virginia, 23185;
C. P. RINSLAND, and M.A.H. SMITH, Atmospheric Sciences Division,
Mail Stop 401A, NASA Langley Research Center, Hampton, Virginia,
23665-5225.

WG6. ABSOLUTE LINE INTENSITIES OF $^{12}CH_3D$ AND PRESSURE BROADENING
COEFFICIENTS FOR CH_3D-N_2 AND CH_3D-H_2 MIXTURES.....15 min.(2:35)

K. P. CARTEN, S. H. KENSINGER, R. W. LOVEJOY, Department of
Chemistry, Lehigh University, Bethlehem, Pennsylvania, 18015;
and C. CHACKERIAN, JR., Astrophysics Experiments Branch,
NASA Ames Research Center, Moffett Field, California, 94035.

Intermission

WG7. TORSIONAL EFFECTS IN THE HAMILTONIAN AND DIPOLE MOMENT OF METHYL SILANE
LIKE MOLECULES.....15 min.(3:05)

N. MOAZZEN-AHMADI and I. OZIER, Department of Physics, University
of British Columbia, Vancouver, British Columbia, Canada, V6T 2A6.

- WG8. THE TORSIONAL SPECTRUM OF CH_3CH_3 AT HIGH RESOLUTION.....15 min.(3:22)
 N. MOAZZEN-AHMADI, H. P. GUSH, M. HALPERN, H. JAGANNATH, A. LEUNG, and I. OZIER, Department of Physics, University of British Columbia, Vancouver, British Columbia, Canada, V6T 2A6. Present address of JAGANNATH: Department of Physics, Alabama A & M University, Normal, Alabama, 35762.
- WG9. TORSIONAL SPLITTINGS IN $\nu_9+\nu_4$ OF C_2H_615 min.(3:39)
 J. SUSSKIND, D. C. REUTER, Laboratory for Atmospheres, NASA/Goddard Space Flight Center, Code 611, Greenbelt, Maryland, 20771; W. E. BLASS, and G. W. HALSEY, Molecular Spectroscopy Laboratory, Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee, 37996.
- WG10. DETERMINATION OF TORSIONAL STATE ROTATIONAL CONSTANTS FROM LOWER STATE COMBINATION DIFFERENCES IN $\nu_9+\nu_4-\nu_4$15 min.(3:56)
 W. E. BLASS, G. W. HALSEY, Molecular Spectroscopy Laboratory, Department of Physics and Astronomy, University of Tennessee, 37996-1200; JOEL SUSSKIND, D. C. REUTER, Laboratory for Atmospheres, NASA/Goddard Space Flight Center, Code 611, Greenbelt, Maryland, 20771; G. W. HALSEY, and D. E. JENNINGS, Laboratory for Extraterrestrial Physics, NASA/Goddard Space Flight Center, Greenbelt, Maryland, 20771.
- WG11. ANALYSIS OF THE 17 μm HIGH RESOLUTION SPECTRUM OF ν_9 OF C_2D_610 min.(4:13)
 F. VILLAMAGNA, S. J. DAUNT, Department of Chemistry, Concordia University, Montreal, Quebec, Canada, H3G 1M8; W. E. BLASS and S. J. DAUNT, Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee, 37996-1200.
- WG12. PRELIMINARY INTERPRETATION OF THE 15 μm SPECTRUM OF ν_{12} OF CH_3CD_310 min.(4:25)
 F. VILLAMAGNA, S. J. DAUNT, Department of Chemistry, Concordia University, Montreal, Quebec, Canada, H3G 1M8; W. E. BLASS, S. J. DAUNT, Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee, 37996-1200; and D. C. REUTER, Laboratory for Atmospheres, NASA/Goddard Space Flight Center, Code 611, Greenbelt, Maryland, 20771.
- WG13. H_2 will be presented here (R. D. SCHAEFFER).....15 min.(4:37)

WEDNESDAY, JUNE 17, 1987 -- 1:30 P.M.

Room 214, Denney Hall

Chairman Before Intermission: T. A. KEIDERLING, Department of Chemistry, University of Illinois at Chicago, Chicago, Illinois.

Chairman After Intermission: GÜNTER GEORG HOFFMANN, Lehrstuhl für Strukturchemie, Ruhruniversität Bochum, D-4630 Bochum, Federal Republic of Germany.

WH1. VIBRATIONAL OPTICAL ACTIVITY OF CHLOROFLUOROACETIC ACID.....15 min.(1:30)

M. A. DAVIES, US Army Ballistic Research Laboratory, Aberdeen Proving Ground, Aberdeen, Maryland, 21005; J. CALIENNI, U. GUNNIA, and M. DIEM, Department of Chemistry, City University of New York, Hunter College, New York, New York, 10021.

WH2. A DEDICATED FOURIER TRANSFORM INSTRUMENT FOR THE MEASUREMENT OF VIBRATIONAL CIRCULAR DICHROISM.....15 min.(1:47)

GÜNTER GEORG HOFFMANN, GÜNTHER SNATZKE, Lehrstuhl für Strukturchemie, Ruhruniversität Bochum, D-4630 Bochum, Federal Republic of Germany; and BERNHARD SCHRADER, Institut für Physikalische und Theoretische Chemie, Universität Essen - GHS, D-4300 Essen, Federal Republic of Germany.

WH3. CH- AND CD-STRETCHING VIBRATIONAL CIRCULAR DICHROISM IN (S,S)-[2,3-²H₂] OXIRANE.....10 min.(2:04)

L. A. NAFIE, T. B. FREEDMAN, M. G. PATERLINI, Department of Chemistry, Syracuse University, Syracuse, New York, 13244; J. M. SCHWAB, and T. RAY, Department of Medicinal Chemistry and Pharmacognosy, School of Pharmacy and Pharmacal Sciences, Purdue University, West Lafayette, Indiana, 47904.

WH4. VIBRATIONAL CIRCULAR DICHROISM SPECTRA OF (S)-4-BENZYL-2-OXAZOLIDINONE IN CDCl₃ SOLUTION.....10 min.(2:16)

R. L. WOOD, T. B. FREEDMAN, and L. A. NAFIE, Department of Chemistry, Syracuse University, Syracuse, New York, 13244.

WH5. VIBRATIONAL CIRCULAR DICHROISM IN THE CH-STRETCHING REGION OF (+)-(3R)-METHYLCYCLOHEXANONE AND CHIRAL DEUTERATED ISOTOPOMERS.....15 min.(2:28)

T. B. FREEDMAN, J. KALLMERTEN, E. D. LIPP, and L. A. NAFIE, Department of Chemistry, Syracuse University, Syracuse, New York, 13244.

WH6. ABSORPTION AND CIRCULAR DICHROISM DUE TO BENDING VIBRATIONS OF A₂B₂ MOLECULES OF C₂ SYMMETRY.....15 min.(2:45)

P. L. POLAVARAPU, Department of Chemistry, Vanderbilt University, Nashville, Tennessee, 37235.

Intermission

WH7. FOURIER TRANSFORM IR-VIBRATIONAL CIRCULAR DICHROISM AND THE PROBLEM OF ARTIFACT SIGNALS.....15 min.(3:15)

P. MALON, Institute of Organic and Biochemistry, Czechoslovak Academy of Science, 16610 Prague 6, CSSR; and T. A. KEIDERLING, Department of Chemistry, University of Illinois at Chicago, Chicago, Illinois, 60680.

WH8. MVCD OF PORPHYRINS AND METALLOPORPHYRINS.....10 min.(3:32)

P. V. CROATTO and T. A. KEIDERLING, Department of Chemistry, University of Illinois at Chicago, Chicago, Illinois, 60680.

WH9. THEORIES OF VIBRATIONAL ROTATIONAL STRENGTHS.....15 min.(3:44)

P. J. STEPHENS, Department of Chemistry, University of Southern California, Los Angeles, California, 90089-0482.

WH10. CALCULATIONS OF VIBRATIONAL ROTATIONAL STRENGTHS.....15 min.(4:01)

P. J. STEPHENS, K. J. JALKANEN, R. W. KAWIECKI, Department of Chemistry, University of Southern California, Los Angeles, California, 90089-0482; R. D. AMOS, N. C. HANDY, Department of Theoretical Chemistry, Cambridge University, Cambridge, United Kingdom; P. LAZZERETTI, and R. ZANASI, Dipartimento Di Chimica, Universita Degli Studi Di Modena, 41,100 Modena, Italy.

WH11. VIBRATIONAL CIRCULAR DICHROISM OF S-(-)-PROPYLENE OXIDE.....15 min.(4:18)

P. J. STEPHENS, R. W. KAWIECKI, F. DEVLIN, Department of Chemistry, University of Southern California, Los Angeles, California, 90089-0482; R. D. AMOS, N. C. HANDY, Department of Theoretical Chemistry, Cambridge University, Cambridge, United Kingdom; and M. A. LOWE, Department of Chemistry, Boston University, Boston, Massachusetts, 02215.

WH12. Π 1 will be presented here (P. LAZZERETTI)15 min.(4:35)

THURSDAY, JUNE 18, 1987 -- 8:30 A.M.

Room 2027, Robinson Laboratory

Chairman: T. AMANO, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada.

RA1. LASER INDUCED FLUORESCENCE SPECTRUM OF COLD METHOXY RADICAL.....15 min. (8:30)

STEPHEN C. FOSTER, XIANMING LIU, PRABHAKAR MISRA, LIAN YU, CRISTINO P. DAMO, and TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

RA2. LASER INDUCED FLUORESCENCE OF FURAN CATION PRODUCED BY MULTIPHOTON IONIZATION IN A SUPERSONIC JET.....15 min. (8:47)

R. S. SMITH, L. F. DIMAURO, Department of Physics, Louisiana State University, Baton Rouge, Louisiana, 70803; and T. J. SEARS, Department of Chemistry, Brookhaven National Laboratories, Upton, New York, 11973.

RA3. LIFETIMES OF THE LOWEST EXCITED STATES OF THE CYCLOPENTADIENYL AND THE MONOMETHYLCYCLOPENTADIENYL RADICALS.....10 min. (9:04)

R. S. SMITH, L. F. DIMAURO, Department of Physics, Louisiana State University, Baton Rouge, Louisiana, 70803; and T. A. MILLER, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

RA4. OPTICAL EMISSION STUDIES ON GRAPHITE IN A LASER/VAPORIZATION SUPERSONIC JET CLUSTER SOURCE.....10 min. (9:16)

M. ANSELMANT, R. S. SMITH, E. DAYKIN, and L. F. DIMAURO, Department of Physics, Louisiana State University, Baton Rouge, Louisiana, 70803.

RA5. LASER INDUCED FLUORESCENCE SPECTRA FROM PHOTOFRAGMENTS OF TOLUENE: A NEW ELECTRONIC TRANSITION OF C₂.....15 min. (9:28)

L. J. VAN DE BURGT, Department of Chemistry, Northwestern University, Evanston, Illinois, 60201; and M. C. HEAVEN, Department of Chemistry, Emory University, Atlanta, Georgia, 30322.

RA6. LASER-INDUCED FLUORESCENCE FROM HCO AND DCO. NEW RESULTS.....15 min. (9:45)

G. RUMBLES, Department of Chemistry, University of California, Irvine, California, 92717; B. STONE, Department of Chemistry, San Jose State University, San Jose, California, 95192; and E.K.C. LEE, deceased.

Intermission

RA7. EVIDENCE FOR A SECONDARY MINIMUM IN THE ArHCl POTENTIAL SURFACE FROM FAR INFRARED LASER/MICROWAVE DOUBLE RESONANCE SPECTROSCOPY OF THE LOWEST ϵ BENDING VIBRATION.....10 min. (10:15)

R. L. ROBINSON, D.-H. GWO, R. J. SAYKALLY, Department of Chemistry, University of California, Berkeley, California, 94720; and D. RAY, Joint Institute for Laboratory Astrophysics and Department of Chemistry, University of Colorado, Boulder, Colorado, 80309.

RA8. MEASUREMENT OF THE VAN DER WAALS STRETCHING VIBRATION IN ArHCl BY FAR INFRARED LASER/MICROWAVE DOUBLE RESONANCE SPECTROSCOPY.....10 min. (10:27)

R. L. ROBINSON, D.-H. GWO, and R. J. SAYKALLY, Department of Chemistry, University of California, Berkeley, California, 94720.

RA9. FAR INFRARED OBSERVATIONS OF HYDROGEN-CONTAINING VAN DER WAALS MOLECULES....15 min. (10:39)

A.R.W. MCKELLAR, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.

RA10. RADICAL VAN DER WAALS MOLECULES.....15 min. (10:56)

WAFAA FAWZY and M. C. HEAVEN, Department of Chemistry, Emory
University, Atlanta, Georgia, 30322.

RA11. STRUCTURES OF N₂O DIMERS AND CLUSTERS FROM FTIR SPECTRA OF N₂O/Ar
SUPERSONIC EXPANSIONS.....15 min. (11:13)

M. GAUTHIER and P. A. HACKETT, Laser Chemistry Group, National
Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.

RA12. DETERMINATION OF THE STRUCTURE OF OCS CO₂.....15 min. (11:30)

S. E. NOVICK, Department of Chemistry, Wesleyan University,
Middletown, Connecticut, 06457; R. D. SUEENRAM, and F. J. LOVAS,
Molecular Spectroscopy Division, National Bureau of Standards,
Gaithersburg, Maryland, 20899.

RA13. Π3 will be presented here (M. A. YOUNG).....15 min. (11:47)

THURSDAY, JUNE 18, 1987 -- 8:30 A.M.

Room 1009, Physics Laboratory

Chairman: WON B. ROH, Department of Engineering Physics, Air Force Institute of Technology, Wright-Patterson AFB, Ohio.

- RB1. ALGEBRAIC APPROACH TO SPECTRA OF SEMI-RIGID POLYATOMIC MOLECULES..... Invited Paper.....30 min.(8:30)

F. MICHELOT, Laboratoire de Spectronomie Moleculaire et Instrumentation Laser, Université de Bourgogne, 2100 Dijon, France.

- RB2. CALCULATION OF HIGH RESOLUTION SPECTRA OF H₂O BY MEANS OF PARTICLES-ON-A-SPHERE MODEL.....10 min.(9:03)

DAVID M. LEITNER, JOHN E. HUNTER, III, R. STEPHEN BERRY, Department of Chemistry, The University of Chicago, Chicago, Illinois, 60637; PABLO VILLARREAL, GERARDO DELGADO-BARRIO, Institute de Estructura de la Materia, C.S.I.C., Madrid-6, Spain; and GRIGORY A. NATANSON, Department of Chemistry, Northwestern University, Evanston, Illinois, 60201.

- RB3. CALCULATION OF THE ROTATIONAL PART OF THE INVERSE OF THE FOUR DIMENSIONAL GENERALIZED TENSOR OF INERTIA OF MOLECULES WITH ONE LARGE-AMPLITUDE INTERNAL MOTION.....15 min.(9:15)

VIKTOR SZALAY, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.

- RB4. INTERNAL ROTATION IN METHYL SILANE: A SEMIRIGID BENDER ANALYSIS.....15 min.(9:32)

R. ESCRIBANO and P. R. BUNKER, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.

- RB5. ABSOLUTE INFRARED INTENSITIES OF FUNDAMENTAL MODES OF H₂O. CALCULATIONS AND EXPERIMENTS WITH MATRIX-ISOLATED H₂O.....².....15 min.(9:49)

M. SZCZESNIAK, K. KUBULAT, RODNEY J. BARTLETT, and WILLIS B. PERSON, Department of Chemistry, University of Florida, Gainesville, Florida, 32611.

- RB6. AB INITIO PREDICTIONS AND INTERPRETATION OF INFRARED SPECTRA OF DERIVATIVES OF H₃PO.....15 min.(10:06)

JOZEF S. KWIAKOWSKI, K. KUBULAT, RODNEY J. BARTLETT, and WILLIS B. PERSON, Department of Chemistry, University of Florida, Gainesville, Florida, 32611.

Intermission

- RB7. THE INFLUENCE OF PRESSURE ON THE NH₃ ν₃ FUNDAMENTAL ABSORPTION SPECTRUM.....10 min.(10:35)

STEVEN A. HENCK and KEVIN K. LEHMANN, Department of Chemistry, Princeton University, Princeton, New Jersey, 08544.

- RB8. ROTATIONAL AND VIBRATIONAL ANALYSIS OF THE 2 N-H STRETCH REGION OF AMMONIA (6700 CM⁻¹).....10 min.(10:47)

STEPHEN L. COY, Department of Chemistry, Harvard University, Cambridge, Massachusetts, 02138; and KEVIN K. LEHMANN, Department of Chemistry, Princeton University, Princeton, New Jersey, 08544.

- RB9. ASSIGNMENT OF THE ν₁+ν₂ AND ν₂+ν₃ BANDS OF THE HIGH RESOLUTION ¹⁴NH₃ FTS ABSORPTION SPECTRA.....15 min.(10:59)

N. TU, G. GUELACHVILI, and K. NARAHARI RAO, Department of Physics, The Ohio State University, Columbus, Ohio, 43210.

RB10. SUBMILLIMETER LASER STARK SPECTROSCOPY OF ND_315 min. (11:16)

R. L. BHATTACHARJEE, G. R. SUDHAKARAN, J. C. SARKER, and
L. H. JOHNSTON, Department of Physics, University of Idaho,
Moscow, Idaho, 83843.

RB11. INFRARED SPECTRA OF UNSTABLE MOLECULES USING THE BURST OF GAS TECHNIQUE.....15 min. (11:33)

T. C. DEVORE, T. R. BURKHOLDER, and T. N. GALLAHER, Department of
Chemistry, James Madison University, Harrisonburg, Virginia, 22807.

RB12. SUBPICOSECOND AMMONIA PHOTODISSOCIATION RATES AS DETERMINED BY RESONANCE
ROTATIONAL HYPER-RAMAN SCATTERING.....10 min. (11:50)

Y. C. CHUNG, J. L. ROEBBER, and L. D. ZIEGLER, Department of Chemistry,
Northeastern University, Boston, Massachusetts, 02115.

THURSDAY, JUNE 18, 1987 -- 8:30 A.M.

Room 1005, Physics Laboratory

Chairman Before Intermission: R. H. TIPPING, Department of Physics and Astronomy, University of Alabama, Tuscaloosa, Alabama.

Chairman After Intermission: R. SOORYAKUMAR, Department of Physics, The Ohio State University, Columbus, Ohio.

- RC1. A REVIEW OF RECENT EXPERIMENTAL STUDIES OF THE INFRARED SPECTRA OF SOLID HYDROGEN ISOTOPES.....INVITED PAPER.....30 min. (8:30)

JAMES R. GAINES, Department of Physics, The Ohio State University, Columbus, Ohio, 43210.

- RC2. ABSORPTION SPECTRA OF SOLID MOLECULAR HYDROGEN IN THE FIRST OVERTONE REGION.....15 min. (9:05)

S. PADDI REDDY, G. VARGHESE, Department of Physics, Memorial University of Newfoundland, St. John's, Newfoundland, Canada, A1B 3X7; and R.D.G. PRASAD, Ranchi University, Ranchi, India.

- RC3. COLLISIONAL INTERFERENCE IN THE PURE ROTATIONAL SPECTRUM OF HD PERTURBED BY FOREIGN GASES.....15 min. (9:22)

P. G. DRAKOPOULOS and G. C. TABISZ, Department of Physics, University of Manitoba, Winnipeg, Manitoba, Canada, R3T 2N2.

- RC4. COLLISION INDUCED ABSORPTION AS A FUNCTION OF TEMPERATURE FOR N₂, CO₂, AND SF₆.....15 min. (9:39)

M. E. THOMAS and M. J. LINEVSKY, Applied Physics Laboratory, The Johns Hopkins University, Laurel, Maryland, 20707.

- RC5. RAMAN SPECTRA OF SOLID MOLECULAR NITROGEN.....15 min. (9:56)

G. GUELACHVILI, Laboratoire d'Infrarouge, Associé au CNRS, Université Paris XI, 91405 Orsay, France, and Department of Physics, The Ohio State University, Columbus, Ohio, 43210; G. PANGILINAN, K. NARAHARI RAO, R. SOORYAKUMAR, Department of Physics, The Ohio State University, Columbus, Ohio, 43210; and R. H. TIPPING, Department of Physics and Astronomy, The University of Alabama, Tuscaloosa, Alabama, 35487.

Intermission

- RC6. RESONANCE RAMAN EXCITATION PROFILES OF Cu(II) CHELATED 1,4-DIHYDROXYANTHRAQUINONE.....15 min. (10:25)

T. S. KOCH and R. P. RAVA, Department of Chemistry, State University of New York at Binghamton, Binghamton, New York, 13901.

- RC7. RESONANCE RAMAN INTERFERENCE IN LINEAR POLYENES.....15 min. (10:42)

I. SZTAINBUCH and G. E. LEROI, Department of Chemistry, Michigan State University, East Lansing, Michigan, 48824.

- RC8. RAMAN TRACE SCATTERING INTENSITY PARAMETERS FOR HYDROCARBONS.....15 min. (10:59)

K. M. GOUGH and W. F. MURPHY, Division of Chemistry, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6.

- RC9. RECENT MEASUREMENTS OF ABSOLUTE INFRARED ABSORPTION INTENSITIES OF LIQUIDS..15 min. (11:16)

JOHN E. BERTIE, H. HARKE, K. AHMED, Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada, T6G 2G2; and H. H. EYSEL, Institut für Anorganische Chemie, der Universität Heidelberg, Heidelberg, West Germany.

- RC10. INFRARED SPECTRA OF ADSORBATES ON ELECTRODE SURFACES.....15 min. (11:33)

MARK W. SEVERSON and P. P. SCHMIDT, Department of Chemistry, Oakland University, Rochester, Michigan, 48063.

- RC11. SURFACE ENHANCED RAMAN STUDY OF BENZIDINE ON Ag ELECTRODE: AN INTERPRETATION FOR DIFFERENT ADSORPTION CONFIGURATIONS AT VARIOUS APPLIED VOLTAGES.....10 min. (11:50)

GUOHAI LIU and GUOZHEN WU, Laboratory of Vibrational Spectroscopy, Institute of Chemistry, Academia Sinica, Beijing, China.

- RC12. FREEZING OF A DIATOMIC FLUID.....10 min. (12:02)

SHERWIN J. SINGER, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210; JOHN D. MCCOY, and DAVID CHANDLER, Department of Chemistry, University of California, Berkeley, California, 94720.

THURSDAY, JUNE 18, 1987 -- 8:30 A.M.

Room 214, Denney Hall

Chairman: CLIFFORD E. DYKSTRA, School of Chemical Sciences, University of Illinois at Urbana-Champaign, Urbana, Illinois.

RD1. THE TRANSFORMATION BETWEEN INTERNAL DISPLACEMENT COORDINATES AND NORMAL COORDINATES OF POLYATOMIC MOLECULES.....10 min. (8:30)

H. C. HSIEH, W. C. ERMILER, and E. R. MALINOWSKI, Department of Chemistry and Chemical Engineering, Stevens Institute of Technology, Hoboken, New Jersey, 07030.

RD2. VIBRATIONAL-ROTATIONAL ANALYSIS OF AB INITIO POTENTIAL ENERGY SURFACES FOR SYMMETRIC-TOP MOLECULES: APPLICATION TO AMMONIA ISOTOPOMERS.....15 min. (8:42)

L. O. HARGISS, Lever Research, Inc., Edgewater, New Jersey, 07020; and W. C. ERMILER, Department of Chemistry and Chemical Engineering Stevens Institute of Technology, Hoboken, New Jersey, 07030.

RD3. HIGH QUALITY CH₂ POTENTIAL ENERGY SURFACES.....15 min. (8:59)

DONALD C. COMEAU and ISALAH SHAVITT, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

RD4. STEREO MUTATION OF METHANE.....15 min. (9:16)

MELANIE J.M. PEPPER and ISALAH SHAVITT, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

RD5. STRUCTURES AND ROTATIONAL CONSTANTS OF C₄O AND C₅O.....10 min. (9:33)

D. W. EWING, Department of Chemistry, John Carroll University, Cleveland, Ohio, 44118.

RD6. STUDY OF THE EFFECTS OF COMPLEX SCALING ON THE CONVERGENCE OF BASIS SET EXPANSION TECHNIQUES AS APPLIED TO THE PROPAGATION OF WAVEPACKETS.....15 min. (9:45)

STEVEN D. PARKER and C. WILLIAM McCURDY, JR., Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

Intermission

RD7. PHOTOIONIZATION CROSS SECTIONS FOR SF₆ BY THE COMPLEX BASIS FUNCTION METHOD.....15 min. (10:15)

CHIN-HUI YU, RUSSELL M. PITZER, and C. WILLIAM McCURDY, JR., Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

RD8. RESTRICTED HARTREE-FOCK WAVEFUNCTIONS AND EXCITATION ENERGIES OF ALKOXY RADICALS.....15 min. (10:32)

STELLA M. SUNG and RUSSELL M. PITZER, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

RD9. POTENTIAL CURVES AND AVOIDED CROSSINGS FOR THE CuF MOLECULE.....15 min. (10:49)

NORA M. WALLACE and RUSSELL M. PITZER, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

RD10. ELECTRONIC STRUCTURE OF URANOCENE.....15 min. (11:06)

AGNES CHANG and RUSSELL M. PITZER, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

RD11. THEORETICAL STUDIES OF DIVALENT VANADIUM IN A MAGNESIUM FLUORIDE HOST.....15 min. (11:23)

N. W. WINTER, Department of Physics, Lawrence Livermore National Laboratory, Livermore, California, 94550; and RUSSELL M. PITZER, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.

RD12. Π8 will be presented here (G. P. Das).....15 min. (11:40)

RD13. Π12 will be presented here (JEFFREY F. GAW).....15 min. (11:57)

THURSDAY, JUNE 18, 1987 -- 1:30 P.M.

Independence Hall Auditorium

SEMINAR OF INVITED PAPERS

IN HONOR OF PROFESSOR WILLIAM GWINN

Chairman: DAVID O. HARRIS, Department of Chemistry, University of California-Santa Barbara, Santa Barbara, California.

- RE1. SPECTROSCOPY ON JULY 4, 1941.....10 min.
RUSSELL M. PITZER, Department of Chemistry, The Ohio State University, Columbus, Ohio, 43210.
- RE2. WILLIAM D. GWINN AND MICROWAVE SPECTROSCOPY IN BERKELEY.....35 min.
ROLLIE J. MYERS, Department of Chemistry, University of California, Berkeley, Berkeley, California, 94720.
- RE3. EQUILIBRIUM STRUCTURES AND PLASMA STARK EFFECTS OF HCO^+ AND RELATED ISOELECTRONIC MOLECULES.....35 min.
R. CLAUDE WOODS, Department of Chemistry, University of Wisconsin, Madison, Wisconsin, 53706.
- Intermission
- RE4. ROTATIONAL SPECTRA AND STRUCTURES OF SMALL CLUSTERS.....35 min.
H. S. GUTOWSKY, School of Chemical Sciences, University of Illinois at Urbana-Champaign, Urbana, Illinois, 61801.
- RE5. HIGH RESOLUTION SPECTROSCOPY OF TRANSITION METAL OXIDES IN THEIR GAS PHASE.....35 min.
TIMOTHY C. STEIMLE, Department of Chemistry, Arizona State University, Tempe, Arizona, 85287.
- RE6. Π_2 will be presented here (P. D. GODFREY).....15 min.(4:29)
- RE7. Π_{10} will be presented here (R. L. ROBINSON).....10 min.(4:46)
- RE8. Π_{11} will be presented here (M. GRUEBELE).....10 min.(4:58)

PLEASE NOTE; THIS SESSION MAY BE MOVED TO PHYSICS 1009 AFTER INTERMISSION.

FRIDAY, JUNE 19, 1987 -- 8:30 A.M.

Room 2027, Robinson Laboratory

Chairman Before Intermission: J. S. MÜJENTER, Department of Chemistry,
University of Rochester, Rochester, New York.

Chairman After Intermission: STEWART NOVICK, National Bureau of Standards,
Gaithersburg, Maryland.

FA1. STATE SELECTIVE PHOTOFRAGMENTATION OF ICl-Ne VAN DER WAALS COMPLEXES.....15 min. (8:30)

JANET C. DROBITS and MARSHA I. LESTER, Department of Chemistry,
University of Pennsylvania, Philadelphia, Pennsylvania, 19104-6323.

FA2. RESONANT PHOTOIONIZATION SPECTROSCOPY OF REFRACTORY METAL-RARE GAS
COMPLEXES.....15 min. (8:47)

JOHN M. GARDNER and MARSHA I. LESTER, Department of Chemistry
and Laboratory for Research on the Structure of Matter, University
of Pennsylvania, Philadelphia, Pennsylvania, 19104-6323.

FA3. OPTOTHERMAL CORRELATION SPECTROSCOPY OF VAN DER WAALS COMPLEXES.....15 min. (9:04)

G. T. FRASER and A. S. PINE, Molecular Spectroscopy Division,
National Bureau of Standards, Gaithersburg, Maryland, 20899.

FA4. SUB-DOPPLER MOLECULAR BEAM SPECTROSCOPY OF TWO COMBINATION BANDS OF
THE CARBON DIOXIDE DIMER.....15 min. (9:21)

R. E. MILLER, K. W. JUCKS, Z. S. HUANG, Department of Chemistry,
University of North Carolina, Chapel Hill, North Carolina, 27514;
G. T. FRASER, A. S. PINE, and W. J. LAFFERTY, Molecular Spectroscopy
Division, National Bureau of Standards, Gaithersburg, Maryland 20899.

FA5. SUB-DOPPLER INFRARED SPECTRUM OF THE CARBON DIOXIDE TRIMER.....15 min. (9:38)

G. T. FRASER, A. S. PINE, W. J. LAFFERTY, Molecular Spectroscopy
Division, National Bureau of Standards, Gaithersburg, Maryland,
20899; and R. E. MILLER, Department of Chemistry, University of
North Carolina, Chapel Hill, North Carolina, 27514.

FA6. SUB-DOPPLER RESOLUTION INFRARED SPECTROSCOPY OF H₂-HF.....15 min. (9:55)

K. W. JUCKS and R. E. MILLER, Department of Chemistry, University of
North Carolina, Chapel Hill, North Carolina, 27514.

FA7. ROTATIONAL PERTURBATIONS IN THE INFRARED SPECTRA OF SEVERAL BINARY
COMPLEXES.....15 min. (10:10)

Z. S. HUANG, K. W. JUCKS, and R. E. MILLER, Department of Chemistry,
University of North Carolina, Chapel Hill, North Carolina, 27514.

Intermission

FA8. INFRARED SPECTROSCOPY AND VIBRATIONAL PREDISSOCIATION OF (HCN)₂ AND
(HCN)₃.....15 min. (10:40)

K. W. JUCKS and R. E. MILLER, Department of Chemistry, University
of North Carolina, Chapel Hill, North Carolina, 27514.

FA9. THE STRUCTURE OF (N₂O)₂ FROM SUB-DOPPLER RESOLUTION NEAR INFRARED
SPECTROSCOPY.....15 min. (10:57)

Z. S. HUANG and R. E. MILLER, Department of Chemistry, University
of North Carolina, Chapel Hill, North Carolina, 27514.

FA10. INFRARED VIBRATION-ROTATION SPECTRUM OF ACETYLENE TRIMER.....15 min. (11:14)

DIANA PRICHARD, J. S. MÜJENTER, Department of Chemistry, University
of Rochester, Rochester, New York, 14627; and B. J. HOWARD,
Physical Chemistry Laboratory, Oxford University, Oxford, OX1 3QZ,
England.

FAL1. INFRARED VIBRATION-ROTATION SPECTRUM OF ARGON-ACETYLENE.....15 min.(11:29)

DIANA PRICHARD, J. S. MÜENTER, Department of Chemistry, University of Rochester, Rochester, New York, 14627; and B. J. HOWARD, Physical Chemistry Laboratory, Oxford University, Oxford, OX1 3QZ, England.

FAL2. INFRARED SPECTRA OF ACETYLENE CLUSTER MOLECULES.....15 min.(11:44)

DIANA PRICHARD, J. S. MÜENTER, Department of Chemistry, University of Rochester, Rochester, New York, 14627; and B. J. HOWARD, Physical Chemistry Laboratory, Oxford University, Oxford, OX1 3QZ, England.

FRIDAY, JUNE 19, 1987 -- 8:30 A.M.

room 1009, Physics Laboratory

Chairman: GARY J. FERLAND, Department of Astronomy,
The Ohio State University, Columbus, Ohio, 43210.

- FB1. VIBRATION-ROTATIONAL INTENSITIES FOR DIATOMIC MOLECULES OF ASTROPHYSICAL INTEREST: THE ISOVALENT MOLECULES CO, CS, SiO AND SiS.....10 min.(8:30)
- R. H. TIPPING, A. LOPEZ PINEIRO, Department of Physics and Astronomy, University of Alabama, Tuscaloosa, Alabama, 35487; and C. CHACKERIAN, JR., NASA Ames Research Center, Moffett Field, California, 94035.
- FB2. DEUTERIUM HYPERFINE STRUCTURE IN INTERSTELLAR CYCLOPROPENYLIDENE-d₁ (C₃HD)..... 5 min.(8:42)
- M. B. BELL, H. E. MATTHEWS, P. A. FELDMAN, L. W. AVERY, J.K.G. WATSON, Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada, K1A 0R6; W. M. IRVINE, and S. C. MADDEN, Department of Physics and Astronomy, University of Massachusetts, Amherst, Massachusetts, 01003.
- FB3. THE INTENSITIES OF HCN OVERTONE TRANSITIONS FROM 12 600 - 18 400 CM⁻¹.....15 min.(8:49)
- A. M. SMITH, Department of Chemistry, Harvard University, Cambridge, Massachusetts, 02138; and K. K. LEHMANN, Department of Chemistry, Princeton University, Princeton, New Jersey, 08544.
- FB4. DIPOLE MOMENTS OF VIBRATIONAL OVERTONE LEVELS OF HCN.....10 min.(9:06)
- J. A. DODD, A. M. SMITH, and W. KLEMPERER, Department of Chemistry, Harvard University, Cambridge, Massachusetts, 02138.
- FB5. PHOSPHINE IN THE 5 μm OBSERVATION WINDOW OF JUPITER: LINE STRENGTHS, H₂- AND He- BROADENED WIDTHS.....15 min.(9:18)
- N. LACOME, A. LEVY, G. TARRAGO, G. POUSSIGUE, and G. GUELACHVILI, Laboratoire d'Infrarouge, Associé au CNRS, Université de Paris-Sud, 91405 Orsay, France.
- FB6. MODELLING OF PHOSPHINE ABSORPTION IN THE 2050-2150 CM⁻¹ JOVIAN WINDOW.....10 min.(9:35)
- G. TARRAGO, G. POUSSIGUE, N. LACOME, A. LEVY, and G. GUELACHVILI, Laboratoire d'Infrarouge, Associé au CNRS, Université de Paris-Sud, 91405 Orsay, France.
- FB7. CLOSED-FORM EXPRESSIONS FOR LOW-TEMPERATURE ROTATIONAL PARTITION FUNCTIONS..10 min.(9:47)
- ROBIN S. McDOWELL, Los Alamos National Laboratory, University of California, Los Alamos, New Mexico, 87545.
- Intermission
- FB8. LOW TEMPERATURE MEASUREMENTS OF PLANETARY GASES.....10 min.(10:10)
- S. NADLER, J. J. HILLMAN, and D. E. JENNINGS, Laboratory for Extraterrestrial Physics, NASA/Goddard Space Flight Center, Greenbelt, Maryland, 20771.
- FB9. INFRARED LINE INTENSITIES OF C10 FROM HIGH RESOLUTION FOURIER TRANSFORM SPECTROSCOPY.....15 min.(10:22)
- J. J. HILLMAN, T. KOSTIUK, J. L. FARIS, and M. J. MUMMA, Laboratory for Extraterrestrial Physics, NASA/Goddard Space Flight Center, Greenbelt, Maryland, 20771.
- FB10. INTENSITIES AND H₂-BROADENED HALF-WIDTHS OF GERMANE LINES AROUND 4.7 μm AT TEMPERATURES RELEVANT TO JUPITER'S ATMOSPHERE.....15 min.(10:39)
- P. VARANASI and S. CHUDAMANI, Laboratory for Planetary Atmospheres Research, State University of New York, Stony Brook, New York, 11794-2300.

FB11. MEASUREMENT OF N_2 -BROADENED LINE WIDTHS OF CO AT LOW TEMPERATURES.....15 min.(10:56)

S. CHUDAMANI, P. VARANASI, and S. KAPUR, Laboratory for Planetary
Atmospheres Research, State University of New York, Stony Brook,
New York, 11794-2300.

FB12. WATER VAPOR CONTINUUM BEYOND 8 MICRONS.....15 min.(11:13)

P. VARANASI, S. CHUDAMANI, and S. KAPUR, Laboratory for Planetary
Atmospheres Research, State University of New York, Stony Brook,
New York, 11794-2300.

*FB13. LINE POSITION MEASUREMENTS OF N_2O AT ELEVATED TEMPERATURES.....10 min.(11:30)

MARK P. ESPLIN and WILLIAM M. BAROWY, Stewart Radiance Laboratory,
Utah State University, Bedford, Massachusetts, 01730.

FB14. LINE STRENGTHS OF THE ν_2 AND ν_4 BANDS OF METHANE.....Arrived Late.....10 min.(11:42)

M. L. LOETE, J. C. HILICO, Laboratoire de Spectrometrie Moleculaire,
Universite de Bourgogne, 21100 Dijon, France; and L. R. BROWN,
Jet Propulsion Laboratory, MS 183-301, 4800 Oak Grove Drive,
Pasadena, California, 91109.

*Already presented as TB15.

FRIDAY, JUNE 19, 1987 -- 8:30 A.M.

Room 1005, Physics Laboratory

Chairman: C. WELDON MATHEWS, Department of Chemistry, The Ohio State University, Columbus, Ohio.

- FC1. AN IMPROVED METHOD FOR THE DIRECT COMPUTATION OF DIATOMIC CENTRIFUGAL DISTORTION CONSTANTS.....15 min. (8:30)
JOEL TELLINGHUISEN, Department of Chemistry, Vanderbilt University, Nashville, Tennessee, 37235.
- FC2. ANALYSIS OF THE D¹-A¹ TRANSITION IN THE EMISSION SPECTRUM OF Cl₂.....15 min. (8:47)
BAOCHUAN GUO, JOEL TELLINGHUISEN, Department of Chemistry, Vanderbilt University, Nashville, Tennessee, 37235; and DILIP K. CHAKRABORTY, Department of Chemistry, University of Nevada at Reno, Reno, Nevada, 89557.
- FC3. TRANSITION STRENGTHS IN THE B-X SYSTEM OF I₂ FROM LINE ABSORPTION MEASUREMENTS.....15 min. (9:04)
JOEL TELLINGHUISEN, Department of Chemistry, Vanderbilt University, Nashville, Tennessee, 37235; DILIP K. CHAKRABORTY, Department of Chemistry, University of Nevada at Reno, Reno, Nevada, 89557; and MARCUS MENDENHALL, Department of Physics, Vanderbilt University, Nashville, Tennessee, 37235.
- FC4. CONSTANTS OF THE 5S 1_g⁺ STATE OF Na₂ FROM TWO-PHOTON SPECTROSCOPY.....15 min. (9:21)
G.-Y. YAN, T. P. DUFFEY, and A. L. SCHAWLOW, Department of Physics, Stanford University, Stanford, California, 94305-4060.
- FC5. SPECTROSCOPIC STUDY OF THE E 1_g⁺ "SHELF" STATE IN ⁷Li₂.....15 min. (9:38)
C. A. TOMCZYK, PPG Industries, Inc. P.O. Box 11472, Pittsburgh, Pennsylvania, 15238; R. A. BERNHEIM, L. P. GOLD, Department of Chemistry, Pennsylvania State University, University Park, Pennsylvania, 16802; and C. R. VIDAL, Max Planck-Institut für Extraterrestrische Physik, D-8046 Garching, Federal Republic of Germany.
- FC6. ZEEMAN EFFECT IN THE DOPPLER-FREE POLARIZATION SPECTROSCOPY OF THE b³π_u STATE OF ⁶Li₂: FINE STRUCTURE CONSTANTS.....15 min. (9:55)
W. H. JENG, Massachusetts Institute of Technology, Room 2069, Cambridge, Massachusetts, 02139; XINGBIN XIE, P.O. Box 110 Dalian, Dalian Liaoning, Peoples Republic of China; L. P. GOLD, and R. A. BERNHEIM, Department of Chemistry, Pennsylvania State University, University Park, Pennsylvania, 16802.
- Intermission
- FC7. ⁶Li-⁷Li ISOTOPE EFFECTS IN THE A¹Σ_u⁺-X¹Σ_g⁺ BAND SYSTEM OF Li₂.....10 min. (10:25)
M. ELSHAKRE, R. A. BERNHEIM, C. M. FAUST, and L. P. GOLD, Department of Chemistry, Pennsylvania State University, University Park, Pennsylvania, 16802.
- FC8. A SPECTROSCOPIC STUDY OF THE 1¹π_g STATE OF ⁷Li₂.....10 min. (10:37)
D. A. MILLER, R. A. BERNHEIM, and L. P. GOLD, Department of Chemistry, Pennsylvania State University, University Park, Pennsylvania, 16802.
- FC9. ACCURATE DISSOCIATION ENERGIES FOR THE X¹Σ⁺ STATES OF KH AND CsH.....15 min. (10:49)
WARREN T. ZEMPE, Department of Chemistry, Wartburg College, Waverly, Iowa, 50677; and WILLIAM C. STWALLEY, Iowa Laser Facility and Departments of Chemistry and Physics, University of Iowa, Iowa City, Iowa, 52242-1294.

- FC10. LASER-INDUCED FLUORESCENCE FROM THE $B^2\Sigma^+$ AND $B'^2\Delta$ STATES OF THE
SiCl RADICAL.....15 min. (11:06)
JAY B. JEFFRIES and RICHARD A. COPELAND, Chemical Physics
Laboratory, SRI International, Menlo Park, California, 94025.
- FC11. THE SPECTRUM OF ZrS.....10 min. (11:23)
R. J. WINKEL, JR., Department of Physics, United States Military
Academy, West Point, New York, 10997-1790.
- FC12. SUB-DOPPLER SPECTROSCOPY OF THE $A^6\Sigma^+-X^6\Sigma^+$ TRANSITION OF MnS.....15 min. (11:35)
M. DOUAY, B. PINCHEMEL, and C. DUFOUR, Laboratoire de Spectroscopie
Moleculaire, Universite de Lille I, 59655 Villeneuve d'Ascq, France.
- FC13. ROTATIONAL ANALYSIS OF THE $A^1\Sigma^+-X^1\Sigma^+$ TRANSITION OF SrS.....10 min. (11:52)
F. S. PIANALTO, C. R. BRAZIER, L. C. O'BRIEN, and P. F. BERNATH,
Department of Chemistry, University of Arizona, Tucson, Arizona,
85721.
- FC14. It will be presented here (G. O. BRINK).....15 min. (12:04)

II SESSION

PLEASE NOTE: The following papers arrived after the program was sent to the printers. The sessions in which they are scheduled for presentation are indicated in the right-hand margin.

- Π1. AN INTERPRETATION OF IR AND VCD INTENSITIES BASED ON NUCLEAR ELECTROMAGNETIC SHIELDINGS.....15 min.(WH12)
P. LAZZERETTI and R. ZANASI, Dipartimento di Chimica, Università degli Studi, Via Campi 183, 41100 - Modena, Italy.
- Π2. ROTATIONAL SPECTRUM AND BENDING POTENTIAL OF LITHIUM HYDROXIDE.....15 min.(RE6)
 D. McNAUGHTON, L. M. TACK, B. KLEIBOMER, and P. D. GODFREY, Chemistry Department, Monash University, Clayton, 3168, Australia.
- Π3. BROADBAND, TIME RESOLVED INFRARED ABSORBANCE SPECTROSCOPY OF TRANSIENT SPECIES.....15 min.(RA13)
R. A. YOUNG and G. C. PIMENTEL, Department of Chemistry, University of California, Berkeley, California, 94720.
- Π4. FREQUENCY STABILIZATION OF A TUNABLE DIODE LASER USING AN INTERNALLY COUPLED CONFOCAL ETALON.....15 min.(WG13)
R. D. SCHAEFFER and W. JALENAK, Spectra Physics, Laser Analytics Division, 25 Wiggins Avenue, Bedford, Massachusetts 01730.
- Π5. DETERMINATION OF THE MOLECULAR STRUCTURE OF SEVERAL CARBO-CATIONS VIA THE 'COULOMB EXPLOSION' TECHNIQUE.....10 min.(TF13)
LESLIE M. TACK, AUREL FAIBIS, ELLIOT P. KANTER, ARGONNE NATIONAL LABORATORY, 9700 S. CASS AVENUE, ARGONNE, ILLINOIS, 60439; and ZEEV VAGER, The Weizmann Institute of Sciences, Rehovot 76100, Israel.
- Π6. STRUCTURAL DETERMINATIONS OF MOLECULAR IONS BY DIRECT THREE-DIMENSIONAL IMAGING: THE 'COULOMB EXPLOSION' EXPERIMENT.....10 min.(TF14)
A. FAIBIS, L. M. TACK, E. P. KANTER, Argonne National Laboratory, 9700 S. Cass Avenue, Argonne, Illinois, 60439; and Z. VAGER, The Weizmann Institute of Science, Rehovot 76100, Israel.
- Π7. STEREOCHEMICAL INFORMATION OF CH_3^+ AND NH_3^+ DERIVED USING THE COULOMB EXPLOSION TECHNIQUE.....10 min.(TF15)
AUREL FAIBIS, Physics Department, Weizmann Institute, Rehovot, Israel; and ELLIOT P. KANTER, LESLIE M. TACK, and J. ZABRANSKY, Argonne National Laboratory, Argonne, Illinois, 60439.
- Π8. THEORETICAL PREDICTION OF CONDUCTIVITY IN DOPED AND UNDOPED POLYMERS.....15 min.(RD12)
G. P. DAS and J. E. MARK, POLYMER RESEARCH CENTER, UNIVERSITY OF CINCINNATI, CINCINNATI, OHIO, 45221.
- Π9. ANOMALOUS POPULATION DISTRIBUTION IN THE $2c \ ^3\Pi_u$ STATE OF MOLECULAR HYDROGEN.....15 min.(FC14)
G. O. BRINK, A. K. BANERJEE, Department of Physics and Astronomy, State University of New York at Buffalo, Amherst, New York, 14260; and K. H. KIM, Department of Physics and Engineering, Hampton University, Hampton, Virginia, 23668.
- Π10. EXTENDED ANALYSIS OF THE BENDING VIBRATION-ROTATION SPECTRUM OF ArHCl BY INTRACAVITY FAR INFRARED LASER/MICROWAVE DOUBLE RESONANCE SPECTROSCOPY.....10 min.(RE7)
R. L. ROBINSON, D.-H. GWO, R. J. SAYKALLY, Department of Chemistry, University of California, Berkeley, California, 94720; and D. RAY, Joint Institute for Laboratory Astrophysics and Department of Chemistry, University of Colorado, Boulder, Colorado, 80309.

- Π11. DIODE LASER VELOCITY MODULATION SPECTROSCOPY OF CARBANIONS; THE C=C
STRETCHING MODE OF ACETYLIDE (C_2H^-).....10 min.(RE8)
M. GRUEBELE, M. POLAK, AND R. J. SAYKALLY, Department of
Chemistry, University of California, Berkeley, California,
94720.
- Π12. AB INITIO HIGHER DERIVATIVES; CUBIC FORCE FIELDS FOR CF_3H , $CClF_2H$,
AND A QUARTIC FORCE FIELD FOR CH_415 min.(RD13)
JEFFREY F. GAW and NICHOLAS C. HANDY, Department of Theoretical
Chemistry, University Chemical Laboratory, Lensfield Road,
Cambridge CB2 1EW, England.

ME1.

(1:30)

INFRARED DETECTION OF HCCCNH⁺: OBSERVATION OF THE ν_1 (N-H STRETCH) FUNDAMENTAL BAND

Sang K. Lee and T. Amano

We report the first observation of the ν_1 (N-H stretch) band of protonated cyanoacetylene (HCCCNH⁺) which is supposed to play an important role in interstellar chemistry by using a difference frequency laser system at NRC. HCCCNH⁺ was generated in a modulated hollow cathode discharge through a gas mixture of HCCCN (~20 mTorr) and H₂ (~400 mTorr). It has been found, however, that the observation should be done at high flow rate of gas mixture to prevent the parent molecule from decomposition. The band origin and the rotational constants have been obtained by a least squares analysis.

Address: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Canada K1A 0R6.

ME2.

(1:42)

INFRARED SPECTROSCOPY OF NH⁺: AN ANALYSIS OF THE PERTURBATION BETWEEN THE X²Π and a⁴Σ⁻ STATES

K. Kawaguchi and T. Amano

NH⁺ is a unique molecule in the sense that it has a very low lying electronic excited state a⁴Σ⁻. It has been known since the first high-resolution UV emission observation by Feast¹ that the energy difference between the X²Π and a⁴Σ⁻ states is only about 500 cm⁻¹ (T_e), and the two states perturb each other strongly. However, no quantitative analyses have been made to unravel the seemingly complicated perturbation.

We have succeeded in observing the v=1 ← 0 transitions in the X²Π and a⁴Σ⁻ states as well as several transitions between the two electronic states in the range of 2450 - 3100 cm⁻¹ with a difference frequency laser. NH⁺ was generated in a hollow cathode discharge through a mixture of NH₃ (~10 mTorr) and He (~1.5 Torr). A least squares fit was performed by including the infrared lines, the term values derived from the electronic emission spectra², and the two FIR lines observed recently³. The molecular constants in the v=1 and 0 states in both the X²Π and a⁴Σ⁻ states were determined precisely.

¹ M.W. Feast, Ap.J. **114**, 344 (1951).

² R. Colin and A.E. Douglas, Can.J. Phys. **46**, 61 (1968).

³ P. Verhoeve, J.J. Ter Meulen, W.L. Meerts, and A. Dymanus, Chem. Phys. Lett. **132**, 213 (1986).

Address of Kawaguchi: Institute for Molecular Science, Okazaki, Japan.

Address of Amano: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Canada K1A 0R6.

ME3.

(1:59)

INFRARED SPECTRUM OF THE ν_3 BAND OF NH_2^+ B. D. REHFUSS, B. M. DINELLI, M. OKUMURA, M. G. BAWENDI, and T. OKA

The ν_3 fundamental vibration-rotation band of NH_2^+ has been observed in the 3μ region with a difference frequency spectrometer as the infrared source and the velocity modulation technique for detection. NH_2^+ was produced in an AC glow discharge with approximately 50 mTorr NH_3 and 6 Torr He.

The spectrum is composed of many triplet lines indicating the electronic symmetry of 3B_1 like the isoelectronic free radical CH_2 . Preliminary analysis shows that NH_2^+ is more quasi-linear than CH_2 in the ground state, which agrees with theoretical predictions on this species¹. More detailed analysis with comparisons to theory will be presented.

¹S. D. Peyerimhoff and R. J. Buenker, *Chemical Physics*, **42**, 167 (1979).

Address of Rehffuss, Okumura, Bawendi and Oka: Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois 60637.

Address of Dinelli: Istituto di Spettroscopia Molecolare del C. N. R., Bologna, Italy.

ME4.

(2:16)

INFRARED SPECTRUM OF THE ν_3 BAND OF NH_3^+ M.G. BAWENDI, B.D. REHFUSS, B.M. DINELLI, M. OKUMURA, and T. OKA

We have observed the vibration-rotation spectrum of the ν_3 band of NH_3^+ . The ion was produced in an air-cooled discharge cell with a gas mixture He : H_2 : NH_3 (600:15:2) and with a total pressure of ≈ 6 Torr. The spectrum was observed using a difference frequency laser system combined with velocity modulation. About 100 lines have been measured and assigned. Spin-rotation splittings for most Q-branch lines were well resolved. A symmetric rotor Hamiltonian with ℓ -resonance and $A_1 - A_2$ splitting was used to analyze the spectrum. We find that NH_3^+ , like the isoelectronic radical CH_3 ,^{1,2} is a planar molecule with D_{3h} symmetry and with an $^2A_2''$ electronic ground state. We obtain the following preliminary vibration-rotation constants (in cm^{-1}):

$\nu_0 - C'\zeta_{33} + \frac{7}{4}\eta_k$	3388.0118(60)		
B^0	10.64500(69)	B'	10.51822(77)
$C'(1 - \zeta_{33}) + \frac{3}{2}\eta_k$	4.67858(108)	$C' - C^0 - 2\eta_k$	-0.05258(100)

Numbers in parentheses are 3σ .

¹G. Herzberg, *Proc. Roy. Soc.* **262A**, 291(1961).

²C. Yamada, E. Hirota, K. Kawaguchi, *J. Chem. Phys.* **75**, 5256(1981).

Address of Bawendi, Rehffuss, Okumura, and Oka: Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois 60637.

Address of Dinelli: Istituto di Spettroscopia Molecolare del C.N.R., Bologna, Italy.

OBSERVATION OF SUB-DOPPLER INFRARED SPECTRUM OF THE H_3O^+ ION

YIT-TSONG CHEN and TAKESHI OKA

The frequency tunable infrared source obtained by using the microwave modulation sidebands on CO_2 laser radiation is sufficiently powerful (5 ~ 10 mWatts) and monochromatic ($\Delta\nu \leq 20$ kHz) to conduct systematic saturation-dip spectroscopy in the 10 μm region. Recently this technique was combined with the multiple reflection mirror system to increase the sensitivity¹ so that it can be applied to molecular ion spectroscopy. We report on the first successful observation of this technique applied to the ν_2 vibration-inversion-rotation transition of H_3O^+ ion. The magnetic field enhanced D.C. negative glow discharge² of ~ 30 mTorr and low current produced the best result. So far the $^9\text{Q}(6,6)$ transition has been observed with the signal to noise better than 10 with linewidth of ~ 500 kHz (FWHM). Using the frequency stabilized CO_2 laser allows us to measure the frequency of the H_3O^+ transition with an absolute accuracy of ≤ 300 kHz. The measurement of more transitions and attempts at observing rotational Zeeman effect and proton hyperfine structure are in progress.

¹Y. T. Chen, J. M. Frye and T. Oka, *J. Opt. Soc. Am.*, **B 3**, 935 (1986).

²F. C. DeLucia, E. Herbst, G. M. Plummer and G. A. Blake, *J. Chem. Phys.*, **78**, 2312 (1983).

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DETERMINATION OF THE DIPOLE MOMENT OF ArH^+ FROM THE ROTATIONAL ZEEMAN EFFECT BY TUNABLE FAR INFRARED LASER SPECTROSCOPY

K. LAUGHLIN, G. A. BLAKE, R. C. COHEN, D. C. HOVDE, AND R. J. SAYKALLY

The first experimental determination of the electric dipole moment of a molecular ion is reported. A tunable far-infrared laser was used to measure the Zeeman effect in low J rotational transitions of ArH^+ and ArD^+ . Using the theory first derived by Townes et al.,¹ the dipole was determined from the isotopic dependence of the rotational g-factors. For ArH^+ and ArD^+ , the current results are: ArH^+ , $g_r = 0.6756(17)$ (1 σ error), ArD^+ , $g_r = 0.3425(14)$, and ArH^+ , $\mu = 1.42(40)$ D (corrected for zero point vibrations). The ultimate accuracy of the method is assessed, considering both the required experimental accuracy and the vibrational dependence of the g-factors.

1. C.H. Townes, G.C. Dousmanis, R.L. White, and R.F. Schwarz, *Disc. Farad. Soc.* **19**, 56 (1955).

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ME7.

(3:07)

THE RENNER TELLER EFFECT IN X $^2\Pi$ CO $_2^+$ *
 J. M. FRYE AND T. J. SEARS

Following work reported at this conference last year and recently published,¹ we have recorded additional infrared spectra of the CO $_2^+$ molecular ion by diode laser absorption spectroscopy. These new spectra originate from vibronic levels associated with the excited bending (ν_2) vibration of the ion and are to levels in the $\nu_2 = 2$ state. Approximately 40 rotation-vibration lines in each of the $^2\Phi + ^2\Delta$ and $(\mu)^2\Pi_{3/2,1/2} + ^2\Sigma^+$ vibronic bands have been detected and assigned at wavelengths between 19 and 22 μm . Many new lines in the ν_2 fundamental bands corresponding to higher rotational excitation have also been recorded. These data make CO $_2^+$ the best documented example of a Renner-Teller interaction in a linear molecule and together with information from the electronic spectrum of the ion, provide a rigorous test of state of the art theory of the effect.

* This research was carried out at Brookhaven National Laboratory under contract DE-AC02-76CH00016 with the U. S. Department of Energy and supported by its Division of Chemical Sciences, Office of Basic Energy Sciences.

¹ T. J. Sears, Mol. Phys. 59, 259 (1986)

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ME8.

(3:30)

VELOCITY MODULATION LASER SPECTROSCOPY OF NEGATIVE IONS: THE INFRARED SPECTRUM OF HYDROSULFIDE (SH $^-$)

M. GRUEBELE, M. POLAK, AND R. J. SAYKALLY

Twenty-five transitions in the $\nu=0+1$ and $\nu=1+2$ bands of $^{32}\text{SH}^-$, as well as in the fundamentals of $^{33}\text{SH}^-$ and $^{34}\text{SH}^-$ have been measured with a diode laser by the velocity modulation technique. The data set was fit to an effective Hamiltonian through sextic terms to determine equilibrium molecular parameters. Comparison with the neutral SH radical shows a strong similarity in the anion and neutral molecular constants, as in the case of OH $^-$. The agreement of experiment with ab initio calculations is found to be quite good.

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ME9.

(3:42)

DIODE LASER VELOCITY MODULATION SPECTROSCOPY OF NEGATIVE IONS: THE ν_3 AND $\nu_3+\nu_2-\nu_2$ BANDS OF THIOCYANATE (NCS $^-$)

M. POLAK, M. GRUEBELE, AND R. J. SAYKALLY

Over 100 absorption lines in the ν_3 and $\nu_3+\nu_2-\nu_2$ bands of NCS $^-$ have been detected using velocity modulation spectroscopy with a diode laser. The ν_3 band origin lies near 2066 cm^{-1} . Additional absorptions have been tentatively assigned to the $\nu_3+\nu_1-\nu_1$ band and should enable determination of the equilibrium moment of inertia.

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ME10.

(3:49)

VELOCITY MODULATION LASER SPECTROSCOPY OF NEGATIVE IONS: THE ν_3 BAND OF AZIDE (N_3^-)

M. POLAK, M. GRUEBELE, AND R. J. SAYKALLY

Thirty-four transitions in the ν_3 (asymmetric stretch) fundamental of the azide anion have been measured in an NH_3/N_2O discharge using diode laser velocity modulation spectroscopy. The data, ranging from P(42) to R(62), were fit to a linear molecule effective Hamiltonian quartic terms. The vibrational band origin was determined to be $\nu_3 = 1986.4672(19) \text{ cm}^{-1}$ and the rotational constants are $B'' = .426203(57) \text{ cm}^{-1}$ and $B' = .422572(55) \text{ cm}^{-1}$. Comparisons with *ab initio* calculations and condensed phase measurements are presented. The observed 2:1 intensity alternation in successive rotational lines establishes the centrosymmetric structure of the anion ($r_0 = 1.188402(82) \text{ \AA}$).

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ME11.

(3:56)

VELOCITY MODULATION INFRARED LASER SPECTROSCOPY OF NEGATIVE IONS: THE ν_3 , $\nu_3+\nu_1-\nu_1$, $\nu_3+\nu_2-\nu_2$ AND $\nu_3+2\nu_2-2\nu_2$ BANDS OF CYANATE (NCO^-)

M. GRUEBELE, M. POLAK, AND R. J. SAYKALLY

132 transitions in the ν_3 (CN stretching) fundamental and the corresponding bending and stretching hotbands of the cyanate anion, ranging from P(52) to R(66), have been measured with a tunable diode laser using the velocity modulation technique. The spectra were fit to the standard linear triatomic molecule rotation-vibration Hamiltonian, yielding effective molecular parameters for the (00 0), (01' 0), (02 0), (10 0), (00 1), (01' 1), (02 1) and (10 1) states. The equilibrium rotational constant was determined to be $B_e = 0.385933(116) \text{ cm}^{-1}$. A comparison with condensed phase results is presented. As previously observed for N_3^- , cyanate is detected with high vibrational excitation in the bending mode, most likely as a consequence of the formation mechanism.

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ME12.

(4:03)

LABORATORY MEASUREMENTS OF THE ABUNDANCE RATIO $[HCO^+]/[HOC^+]$ AND THEIR ASTROPHYSICAL IMPLICATIONS

T. Amano and T. Nakanaga

Recently the ν_1 fundamental band of HOC^+ was observed in a hollow cathode discharge through a mixture of CO and H_2 .¹ The reaction condition is quite a contrast to that used in previous microwave observations in which a large amount of Ar is needed as a buffer gas.

The relative intensity of the infrared absorption lines of HCO^+ and HOC^+ was measured as a function of the pressures of H_2 and CO. In the laboratory conditions, the isomerization of HOC^+ to HCO^+ by CO was found to be a dominant depletion process of HOC^+ . The abundance ratio $[HCO^+]/[HOC^+]$ was obtained to be about 220 under the most favorable reaction conditions for production of HOC^+ . Although the rate constant of the catalytic isomerization of HOC^+ by H_2 is smaller than that of the isomerization reaction by CO by about an order of magnitude, the catalytic isomerization by H_2 may be the main depletion process of HOC^+ in dense dark clouds. The estimated rate constants derived in the present work gives an estimated abundance ratio $[HCO^+]/[HOC^+]$ to be of the order of 10^5 in dense dark clouds.

¹ T. Nakanaga and T. Amano, Paper FA15, 41st Symposium on Molecular Spectroscopy and J. Mol. Spectrosc. to be published.

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ME13.

(4:20)

OBSERVATION OF THE ν_1 AND ν_3 FUNDAMENTAL BANDS OF H_2Cl^+

Sang K. Lee, T. Amano, M. Oldani, and K. Kawaguchi

The ν_1 and ν_3 bands of chloronium ion (H_2Cl^+) have been observed with a difference frequency laser system at NRC. The ion was generated through a hollow cathode discharge modulated at 16 kHz in a gas mixture of HCl (~30 mTorr) and H_2 (~0.7 Torr). The observation was done with a dry-ice cooled multiple traversal cell connected to a fast flow pumping system.

The assignment was not easily made due to the Coriolis interaction between the $\nu_1 = 1$ and $\nu_3 = 1$ states. The first clue of the assignment was obtained by a systematic sorting for the ground state combination differences which were known from the analysis of the ν_2 band by Kawaguchi and Hirota.¹ A least squares fit of the observed transitions has been done by employing Watson's A-reduced Hamiltonian, and the band origins, rotational constants, and centrifugal distortion constants have been obtained.

¹ K. Kawaguchi and E. Hirota, *J. Chem. Phys.* **85**, 6910 (1986).

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ME14.

(4:37)

THE ν_1 AND ν_3 FUNDAMENTAL BANDS OF SH_3^+

T. Nakanaga and T. Amano

We reported a preliminary analysis of the ν_3 fundamental band of SH_3^+ at this meeting a year ago¹. The vibration-rotation levels in the $\nu_3 = 1$ state were found perturbed. The molecular constants in the $\nu_3 = 1$ state were obtained by excluding the severely perturbed lines, whereas the ground state constants were well determined by using the combination differences.

Ab initio calculations have predicted that the ν_1 fundamental band lies very close to the ν_3 fundamental band within several cm^{-1} . The assignments of the ν_1 fundamental, however, had not been easily done presumably due to much smaller intensity, until a systematic sorting of the ground state combination differences was performed on all the unassigned lines. A simultaneous analysis of the ν_1 and ν_3 bands was made by including the higher-order vibration-rotation interaction terms ($\Delta(K, \ell) = \pm 3$), and the molecular constants were determined for the $\nu_1 = 1$ and $\nu_3 = 1$ states.

¹ T. Nakanaga and T. Amano, Paper FA5, 41st Symposium on Molecular Spectroscopy and Chem. Phys. Lett. to be published.

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Address of Amano: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Canada K1A 0R6.

INITIAL ASSIGNMENT OF THE PROTONATED ACETYLENE VIBRATION-ROTATION SPECTRUM

M. W. CROFTON, M.-F. JAGOD, B. D. REHFUSS, and T. OKA

Two years ago we reported the observation of a rich vibration-rotation spectrum of carbon cation transitions in the CH stretching region. Some of these lines were found to be due to the ν_3 fundamental band of CH_3^+ and its analysis has been completed.¹ Subsequently, another group of lines has been assigned to the C_2H_2^+ ion.² From chemical evidence and the unusual appearance of the spectrum, the remaining prominent features were presumed to be produced by C_2H_3^+ . This presumption is now supported by the agreement of the observed spectral pattern with that calculated for nonclassical protonated acetylene on the basis of Hougen's approximate internal rotation model.³ To make the first tentative assignments, the model parameters were adjusted to approximate the observed spectrum. As of this writing, more than 30 lines have been tentatively assigned. The first attempts to fit the spectrum using the approximate Hamiltonian employed for Hougen's model will be described. While there are questions about individual assignments, we are confident about the basic structure of the overall assignment.

¹M. W. Crofton, M.-F. Jagod, B. D. Rehfuss, W. A. Kreiner, and T. Oka, *J. Chem. Phys.*, **83**, 3702 (1985).

²M.-F. Jagod, M. W. Crofton, B. D. Rehfuss, and T. Oka, 42nd Symposium on Molecular Spectroscopy, Columbus, Ohio.

³J. T. Hougen, *J. Mol. Spectrosc.*, **122**, (1987), in press.

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Address of Jagod, Rehfuss, and Oka: Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois 60637.

INFRARED SPECTRUM OF THE ν_3 BAND OF C_2H_2^+

M.-F. JAGOD, M. W. CROFTON, B. D. REHFUSS, and T. OKA

We have observed the ν_3 fundamental vibration-rotation band of C_2H_2^+ ($^2\Pi_u$). This band was among the very rich hydrocarbon spectra in the $3.3 \mu\text{m}$ region which also yielded the spectra of CH_3^+ and C_2H_3^+ .² It was observed using a difference frequency spectrometer and velocity modulation for detection. This ion was produced in an AC glow discharge with a gas mixture of He : H_2 : C_2H_2 (700:20:1) with a total pressure of ≈ 6 Torr. The spectral lines of C_2H_2^+ could be discriminated from those of CH_3^+ and C_2H_3^+ by their different chemical behavior. We have determined the preliminary molecular constants as³ (in cm^{-1}):

ν_0	3135.975(5)		
B_0	1.10456(7)	B'	1.09895(13)
D_0	1.44×10^{-6}	D'	1.44×10^{-6}
A_0	-30.1(15)	A'	-29.6(15)
AD_0	$1.7(34) \times 10^{-3}$	A'_D	$3.3(35) \times 10^{-3}$

Numbers in parentheses are 3σ .

¹M. W. Crofton, M.-F. Jagod, B. D. Rehfuss, W. A. Kreiner, and T. Oka, *J. Chem. Phys.*, **83**, 3702 (1985).

²M. W. Crofton, M.-F. Jagod, B. D. Rehfuss, and T. Oka, 42nd Symposium on Molecular Spectroscopy, Columbus, Ohio.

³M. W. Crofton, M.-F. Jagod, B. D. Rehfuss, and T. Oka, *J. Chem. Phys.*, **86**, (1987), in press.

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MF1.

(1:30)

THE VIBRATIONAL AND ROTATIONAL SPECTRA OF OZONE FOR THE (0,1,0) AND (0,2,0) STATES

**H. M. PICKETT, E. A. COHEN, L. R. BROWN, C. P. RINSLAND, M. A. H. SMITH,
V. MALATHY DEVI, A. GOLDMAN, A. BARBE, B. CARLI, AND M. CARLOTTI**

The rotational frequencies of the (0,1,0) and (0,2,0) states and line positions of the ν_2 and $2\nu_2 - \nu_2$ bands of the normal isotope of ozone have been fitted through $J = 65$ and $K = 21$ to three-state Hamiltonian using new measurements in the microwave, far infrared and $600\text{--}850\text{ cm}^{-1}$ infrared regions. The rms. error in the fit is 0.05 MHz for the microwave lines and 0.0006 cm^{-1} for the far infrared and infrared lines. In addition, intensities of 497 lines of ν_2 through $J = 49$ and $K = 14$ and 45 lines of $2\nu_2 - \nu_2$ through $J = 32$ and $K = 4$ have been fitted to the transition dipole and 4 interaction terms. Large intensity perturbations are observed due to mixing of the large permanent and ν_3 dipoles with the smaller ν_2 dipole. Comparison with theory shows that the rotational and fundamental vibrational intensities form a self-consistent set within an experimental uncertainty of 4% and are consistent with ultraviolet absorption determinations.

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MF2.

(1:47)

INTENSITIES AND ANALYSIS OF THE $\nu_1 + \nu_2$ AND $\nu_2 + \nu_3$ BANDS OF $^{16}\text{O}_3$ NEAR $5.7\ \mu\text{m}$

V. MALATHY DEVI, J.-M. FLAUD, C. CAMY-PEYRET, C. P. RINSLAND, AND M. A. H. SMITH

Spectra of ozone generated from a >99.98% pure oxygen sample were recorded covering the 4.5 to $10\ \mu\text{m}$ region at 0.005 cm^{-1} resolution with the McMath Fourier transform interferometer at the National Solar Observatory on Kitt Peak. An extensive analysis of the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ bands in the $5.7\text{-}\mu\text{m}$ region was performed using spectra recorded with about 10.3 and 23.7 Torr of ozone in a 50-cm long absorption cell. Using the results reported in a previous study¹, initial assignments involving low and medium J and K_a values ($J \approx 45$, $K_a \approx 11$) were made, and a first calculation performed using a Hamiltonian taking into account the Coriolis-type interaction between the rotational levels of the (110) and (011) vibrational states. From this initial set of constants an improved set of vibrational, rotational, and coupling constants was obtained which helped to extend the assignments to higher J and K_a transitions. The process was repeated until almost all of the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ lines observable in the laboratory spectra were assigned, thus extending the quantum number assignments to $J \leq 57$, $K_a \leq 16$ for the $\nu_1 + \nu_2$ band and $J \leq 55$, $K_a \leq 15$ for the $\nu_2 + \nu_3$ band.

Using the equivalent width method, about 220 line intensities were measured with an average relative uncertainty of 10%. Because the exact amount of ozone in the cell was not known, intensities of lines in the ν_1 and ν_3 bands near $10\ \mu\text{m}$ were also measured in the same spectrum and compared to calculated values² to calibrate the measurements onto an absolute intensity scale. Precise transition moment constants were then deduced for both bands from these values. From the vibrational energies, rotational, and coupling constants, as well as the transition moment constants, a list containing 7110 line positions and intensities for the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ bands of ozone has been generated. Total band intensities of 0.237×10^{-19} and $0.536 \times 10^{-19}\text{ cm}^{-1}/\text{molecule cm}^{-2}$ at 296 K were obtained respectively for the $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ bands.

Numerous weak lines believed to belong to the $2\nu_2 + \nu_3 - \nu_2$ and the $2\nu_1 + \nu_2 - \nu_2$ hot bands were also observed in the spectra. Analysis of these features has not been attempted at this time.

¹ A. Barbe, C. Secroun, P. Jouve, C. Camy-Peyret, and J.-M. Flaud, *J. Mol. Spectrosc.*, **75**, 103 (1979).

² J.-M. Flaud, C. Camy-Peyret, V. Malathy Devi, C. P. Rinsland, and M. A. H. Smith, *J. Mol. Spectrosc.*, in press.

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MF3.

(1:59)

PRESSURE-INDUCED LINE SHIFTS AND WIDTHS OF O_3 BROADENED BY N_2 AND BY AIR

M. A. H. SMITH, V. MALATHY DEVI, C. P. RINSLAND, AND D. CHRIS BENNER

Fourier transform spectra of O_3 broadened by approximately 100 to 300 Torr N_2 or dry air have been analyzed to determine both halfwidths and shifts for over 60 lines in the 9- μ m region. The spectra were recorded at 0.005 cm^{-1} resolution with the McMath FTS at the National Solar Observatory on Kitt Peak, and halfwidths and line positions were determined using a nonlinear least-squares spectral fitting technique. Unshifted line positions were determined from additional FTS spectra of nearly pure O_3 at low pressure, and all spectra were calibrated using well-known H_2O lines near 7.5 μ m. Additional broadening measurements were made for 13 of the O_3 lines using the tunable diode laser spectrometer at NASA Langley Research Center. The TDL results agree with the FTS measurements within 4%.

Most of the lines measured belong to the R branch of the ν_1 band of O_3 , covering the range of rotational quantum numbers $8 \leq J'' \leq 45$ and $0 \leq K''_a \leq 11$. For both air and N_2 broadening, the majority of observed halfwidths fall within the range 0.065 to $0.09\text{ cm}^{-1}\text{ atm}^{-1}$, and the shifts vary between $+0.004\text{ cm}^{-1}\text{ atm}^{-1}$ and $-0.008\text{ cm}^{-1}\text{ atm}^{-1}$. A strong dependence on rotational quantum numbers J'' and K''_a is observed for both halfwidths and shifts.

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MF4.

(2:11)

THE PURE ROTATIONAL SPECTRUM OF $^{14}N^{16}O_2$

A. PERRIN, J.-M. FLAUD, C. CAMY-PEYRET, B. CARLI AND M. CARLOTTI

The pure rotation spectrum of NO , between 8 and 200 cm^{-1} has been recorded at an unapodized resolution of 0.0033 cm^{-1} using the Fourier transform spectrometer of IROE. This spectrum has been completely analyzed leading to an extensive and precise set of spin rotation levels (up to $N=50$ and $K=13$) for the ground state. Then, using a computer program which fully treats the spin-rotation interaction, it has been possible to reproduce to their experimental uncertainty the experimental levels and to determine an improved set of spin-rotation and rotational constants for the ground state of $^{14}N^{16}O_2$.

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MF5.

(2:23)

ANALYSIS OF THE 3 μm BANDS OF BENZENE

J. PLÍVA AND A. S. PINE

A comprehensive rovibrational analysis is reported for the 3 μm absorption bands of the benzene molecule measured on a difference-frequency laser spectrometer and deconvolved to an effective linewidth of 0.0010 - 0.0015 cm^{-1} . The four strong bands observed, centered at 3047.908, 3078.614, 3100.408, and 3101.854 cm^{-1} , are due to the E_{1u} fundamental ν_{12} sharing its intensity with the E_{1u} components of the states $\nu_{13}+\nu_{16}$, $\nu_2+\nu_{13}+\nu_{18}$, and $\nu_3+\nu_{10}+\nu_{18}$ via anharmonic resonances. The bands exhibit strong perturbations due to l-resonances with the inactive B_{1u}/B_{2u} components of the $\nu_{13}+\nu_{16}$ and $\nu_2+\nu_{13}+\nu_{18}$ states, and numerous localized perturbations due to overtones and combinations of the 16 low frequency vibrations of the molecule. Symmetry arguments and values of constants such as C_I known for the fundamentals have been used to propose tentative assignments for many of the perturbing states.

A Hamiltonian matrix containing all components of the main interacting states plus 18 perturbing states was used for the treatment of ~8400 assigned transitions. A set of spectroscopic constants is reported which reproduces all the data with a standard deviation of 0.0012 cm^{-1} . It is found that x,y-Coriolis and anharmonic resonances of surprisingly high order have to be invoked to account for most of the localized perturbations observed in the spectrum.

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MF6.

(2:40)

HIGH RESOLUTION FOURIER TRANSFORM SPECTRUM OF DISULFANE, H_2S_2 , BETWEEN 30 AND 90 cm^{-1}

G.M. Plummer, G. Winnewisser, B.P. Winnewisser, and M. Winnewisser

The rotational spectrum of disulfane has been recorded between 30 and 340 cm^{-1} with a resolution of approximately 0.0025 cm^{-1} . These measurements were carried out in the HRFTS Laboratory at the Justus-Liebig-Universität in Gießen in a new absorption cell specially designed for such quasi-stable molecules, and provide a text-book example of the perpendicular spectrum of a nearly prolate rotor. The assignment and analysis of a large number of features up to 90 cm^{-1} will be presented.

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MF7.

(3:10)

EXTENSIVE VIBRATIONAL STATE MIXING OF INDIVIDUAL ROTATIONAL LEVELS IN 1-BUTYNE NEAR 3333 cm^{-1}

A. N. DE SOUZA, DEVINDER KAUR, AND D. S. PERRY

An infrared absorption spectrum of jet-cooled (3K) 1-butyne is recorded by monitoring the attenuation of a scanned single-mode F-center laser beam. Rigorous assignments are made by comparison of combination-differences with microwave data on this near-prolate asymmetric top. Levels with $K_{-1}=0$ are heavily mixed for all J and appear as a clump of 4 or more. The density of coupled states approximates the calculated total density of vibrational states (~ 60 per cm^{-1}). The $K_{-1}=1$ levels are apparently unperturbed for $J \leq 3$ but heavily mixed for higher J (≥ 7). The little information available on $K_{-1}=2$ indicates that it is strongly mixed even for low J . As compared to $K_{-1}=0, 2$, $K_{-1}=1$ is anomalously noninteractive with the bath of vibrational levels. From a kinetic point of view, the data provide a detailed picture of collisionless intramolecular vibrational redistribution (IVR) in the energy region where it is "turning on".

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MF8.

(3:27)

ASSIGNMENT OF CH_3OH FIR LASER LINES FROM NON-CO-STRETCH STATES

I. MUKHOPADHYAY, M. MOLLABASHI, W. LEWIS-BEVAN, J.W.C. JOHNS AND R.M. LEES

Assignments of far-infrared (FIR) laser lines of CH_3OH originating from excited states other than the normal CO-stretch mode will be discussed. First, laser lines optically pumped by the 9R(18), 10P(12) and 13-9R(18) CO_2 laser lines will be examined. It is proposed that each of these FIR laser systems involves highly excited $n=3$ torsional levels of the ground vibrational state, in two cases interacting via Fermi resonance with $n=0$, C-O stretch levels. Secondly, FIR emission from CH_2 deformation and CH_3 in-plane rocking modes, pumped by the 9P(40), 10R(44), 13-9P(14) and 13/18-9P(34) CO_2 lines, will be considered. Probable assignments will be presented, along with supporting spectroscopic evidence from combination frequency loops formed from observed or calculated IR and FIR frequencies.

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MF9.

(3:44)

LASER STARK SPECTRA OF $^{13}\text{CH}_3\text{OH}$ AT $311\mu\text{m}$ AND $337\mu\text{m}$

G. R. SUDHAKARAN, L. H. JOHNSTON, J. SARKER, AND R. BHATTACHARJEE

The laser Stark spectra of $^{13}\text{CH}_3\text{OH}$ have been observed using the $311\mu\text{m}$ and the $337\mu\text{m}$ line of the HCN Laser. Numerous families of absorptions have been observed for both π and σ polarizations all the way up to $60,000\text{ V/cm}$. The low field structure observed with the $311\mu\text{m}$ line is assigned to the $J_K = 15_3 + 14_2\text{ A}^- \nu_t = 0$ torsional state. One of the several prominent structures seen with the $337\mu\text{m}$ line is tentatively identified as the $J_K = 22_6 + 22_5\text{ E}_1 \nu_t = 0$ transition.

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MF10.

(3:56)

ON THE ASSIGNMENT OF THE HIGH EFFICIENCY 127 μm FIR LASER LINE OF $^{13}\text{CD}_3\text{OH}$ AND OTHER CH_3OH , CD_3OH AND CD_3OD FIR LASER LINES

I. MUKHOPADHYAY, M. MOLLABASHI, W. LEWIS-BEVAN AND R.M. LEES

An assignment is proposed for the strong 127.02 μm $^{13}\text{CD}_3\text{OH}$ far-infrared (FIR) laser line, which was recently reported by Inguscio et al. (1) to be pumped with very high efficiency by the 10P(8) CO_2 laser line. On the basis of several spectroscopic clues derived from calculated energies and molecular parameters for $^{13}\text{CD}_3\text{OH}$, this line is identified as the $(n\tau K, J) = (116, 17) \rightarrow (125, 16)$ transition, and its companion 462.8 μm FIR line as the $(116, 17) \rightarrow (116, 16)$ transition. In addition, assignments will be proposed for a number of other reported FIR laser lines for this species and for CH_3OH , CD_3OH and CD_3OD , with supporting spectroscopic evidence and frequency combination loops.

(1) M. Inguscio, K.M. Evenson, F.R. Petersen, F. Strumia, and E. Vasconcellos, Int. J. IR and MM Waves 5, 1289-1296 (1984).

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MF11.

(4:13)

LASER STARK SPECTROSCOPY OF CD_3OD AT 337 μm WITH THE HCN LASER

J. C. SARKER, L. H. JOHNSTON, G. R. SUDHAKARAN, R. L. BHATTACHARJEE

Laser Stark spectra have been observed between the 337 μm line of the HCN laser and the Stark-shifted spectrum of fully deuterated methyl alcohol (CD_3OD). Numerous families of absorptions have been found in both parallel and perpendicular polarizations. A relatively strong transition which shows up at high field has been assigned as the $J_K = 9_7 + 8_6 A$, $v_t = 0$ torsional state. The other two families originating at low field have tentatively been identified as the $J_K = 18_3 + 17_2$ F_1 , $v_t = 0$ and $J_K = 17_3 + 16_4$ E_1 , $v_t = 1$ torsional state.

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MF12.

(4:30)

FREE JET INFRARED ABSORPTION SPECTROSCOPY OF THE ν_6 AND ν_7 BANDS OF IRON PENTACARBONYL

YOSHIYASU MATSUMOTO, TETSURO MAJIMA, AND MICHIO TAKAMI

The infrared diode laser absorption spectra of ν_6 (CO stretching, 2038.10 cm^{-1}) and ν_7 (CO bending, 619.94 cm^{-1}) bands of $\text{Fe}(\text{CO})_5$ have been studied in a supersonic free jet. Owing to several low frequency vibrational modes, the vibrational level density at $\nu_6=1$ is as high as $\sim 5 \times 10^4/\text{cm}^{-1}$, while the density at $\nu_7=1$ is only $\sim 20/\text{cm}^{-1}$. In spite of the large difference in background vibrational level density, both bands show the similar rotational structure characteristic to the parallel band of symmetric top molecules.

The larger linewidth observed in the ν_6 band is attributed to the inhomogeneous broadening inherent to the spatial inhomogeneity in a free jet. The influence of the dense background levels to the ν_6 band is found to be a minor effect.

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MF13.

(4:47)

INFRARED BAND STRENGTH MEASUREMENTS OF CF_2 J. WORMHOUDT

The absolute strengths of the fundamental absorption bands of the CF_2 molecule have been predicted,¹ but no measurements have been made. We have investigated the strength of the ν_3 band using a tunable diode laser to measure individual line strengths. Experiments were performed in a flow tube using a multipass cell. Two methods were used to quantify the CF_2 flow. In the first, CF_2HCl was thermally decomposed in an internal oven, and HCl infrared absorption was used as a measure of the column density of CF_2 . In the second, a tunable dye laser was used to measure absorption in the $\tilde{A}^1\text{B}_1-\tilde{X}^1\text{A}_1$ electronic band, for which peak absorption cross sections have been measured.² Results of both techniques will be discussed.

¹J.H. Newton and W.B. Person, J. Chem. Phys. 68, 2799 (1978).

²D.S. King, P.K. Schenck, and J.C. Stephenson, J. Mol. Spec. 78, 1 (1979).

Work supported by AFOSR under Contract F49620-84-C-0036.

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MF14.

(4:59)

OBSERVATION AND ANALYSIS OF THE XeF_2 1030 cm^{-1} BANDSRICHARD W. SCHWENZ AND D. J. DONALDSON

The infrared spectrum of XeF_2 is observed using a Fourier transform infrared spectrometer at 0.02 cm^{-1} resolution. At this resolution we are able to rotationally resolve the $0^1_10 \rightarrow 2^1_10$ and either 0^2_20 or $0^0_01 \rightarrow 2^0_01$ bands.

The information obtained in this experiment is combined with previous infrared¹ and Raman^{2,3} studies of lower vibrational states to determine rovibrational constants for the ground state of the XeF_2 molecule.

¹S. Reichman and F. Schreiner, J. Chem. Phys., 51 (1969) 2355.

²P. Tsao, C. Cobb and H. Claassen, J. Chem. Phys., 54 (1971) 5247.

³N. Brassington, H. Edwards and D. Long, J. Chem. Soc. Faraday II, 74 (1978) 1208.

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MG1.

(1:30)

MICROWAVE SPECTRUM AND STRUCTURE OF CYCLOBUTENE OZONIDE AND CYCLOBUTADIENE OZONIDE

P. LORENČAK, H. BADAWI, D. BORSETH, G.D. MENDENHALL, K.W. HILLIG, II, AND R.L. KUCZKOWSKI

¹⁸O Cyclobutene ozonide (2,3,7-trioxabicyclo[2.2.1]-heptane) containing D and ¹⁸O enrichment was prepared by ozonolysis of cyclobutene and by singlet oxygen addition to furan. From the assignment of four isotopic species, it was established that the ozonide has C_s symmetry. The peroxy bond distance is 1.489(1)Å which is elongated about 0.03Å compared to less strained monocyclic ozonides. The singlet oxygen synthesis also leads to cyclobutadiene ozonide (2,3,7-trioxabicyclo[2.2.1]-hept-5-ene). This species was recently isolated and its MW spectrum (normal species) was assigned. The current status of its analysis will be discussed.

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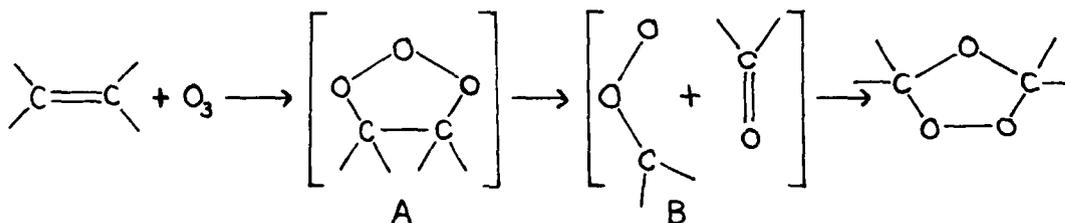
MG2.

(1:42)

MILLIMETER WAVE SPECTRUM OF THE PRIMARY OZONIDE OF ETHYLENE

J. ZOZOM, R. D. SUENRAM, C. W. GILLIES, AND F. J. LOVAS

The reaction of ozone with olefins is one of the major reaction pathways responsible for the formation of photochemical smog in the troposphere over major urban areas. Because of this, much work has gone into the elucidation of the reaction mechanism. From this previous work the reaction sequence is thought to proceed as outlined below:



In all of the previous experimental work the primary ozonide (A), and the Criegee intermediate (B) have never been observed in solution or gas phase experiments although they are both thought to be key intermediates in the overall reaction scheme. Their existence has only been inferred from secondary chemical evidence involving chemical trapping and end product analysis.

Now, for the first time, the primary ozonide (A) has been observed in the prototypical reaction of ozone with ethylene, the smallest olefin. The rotational spectra of six isotopic species have been observed at -100°C using a specially designed low temperature absorption cell. The free molecule in the gas phase exhibits an envelope type of structure with the central oxygen forming a 50° out of plane "flap" of the five membered heavy atom ring. Details of the structural determination and the dipole moment analysis will be presented.

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MG3.

(1:59)

ROTATIONAL SPECTRA OF ^{13}C TAGGED PROPYNE IN THE ν_{10} VIBRATION

J. A. ROBERTS, I. AN, AND H. TAM

A study was made of the propyne and acetonitrile molecules on the rotational spectral components, $0 \leq J \leq 4$, in low lying vibrational levels. Both the ^{12}C and isotopically substituted species of ^{13}C in CH_3CCH and CH_3CN molecules were studied. Recent studies on these two molecules in vibrational levels had shown strong resonance interactions within vibrations and combination vibration bands which do not appear to be explained by simple perturbation models. A study of the isotopically substituted components appeared to be promising.

A comprehensive model was developed for the $^{12}\text{CH}_3^{12}\text{C}^{12}\text{CH}$ molecule and from the experimental results some resonance interactions were found which could be explored further by use of isotopic shifts in the spectra. We have been able initially to study the molecules $^{13}\text{CH}_3^{12}\text{C}^{12}\text{CH}$, $^{12}\text{CH}_3^{13}\text{C}^{12}\text{CH}$ and $^{12}\text{CH}_3^{12}\text{C}^{13}\text{CH}$ in the $\nu_{10} = 1$ and ground vibration for naturally abundant ^{13}C . Thus far, the comprehensive model developed for this ^{12}C species appears to hold but data are limited.

Spectral studies made upon rotational components in the $\nu_{10} = 1, 2, 3$ and 4 vibrations of CH_3CCH and rotational components of the $\nu_8 = 1, 2,$ and 3 vibrations of $\text{CH}_3\text{C}^{14}\text{N}$ and $\text{CH}_3\text{C}^{15}\text{N}$ indicated a departure from a molecular model based upon perturbation techniques but these results were used successfully to predict a number of components in the isotopic species.

The major thrust of this paper is to present accurate experimental data for $\Delta J = +1$ rotations for $1 \leq J \leq 4$ in the frequency range 15 to 95 GHz and for the $\nu_{10} = 1$ for each isotope of propyne and for the $\nu_8 = 1$ and 2 for the acetonitrile isotopes.¹⁰ From these data we have produced a molecular model which shows the trend in each molecular parameter with quantum number $\nu, J, K,$ and ℓ .

1. This work supported by Grant #B-842 The Robert A. Welch Foundation, Houston, TX.

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MG4.

(2:11)

MICROWAVE SPECTRUM OF BIS-TRIFLUOROMETHYL NITROXIDE

R. M. WHITE AND J. D. GRAYBEAL*

The high resolution microwave spectrum of the stable radical bis-trifluoromethyl nitroxide, $(\text{CF}_3)_2\text{NO}$, has been observed in the region from 18-26.5 GHz. The rotational constants determined by calculation of the hypothetical unsplit rotational transitions and use of the Kirchoff NBS fitting program¹ are: $A = 2256.94$, $B = 1056.08$, and $C = 971.51$ MHz.

Using the irreducible tensor technique to evaluate the nonvanishing matrix elements, the analysis of the hyperfine structure of 9 separate transitions yielded spin-rotation coupling constants of $E_{aa} = -35.98$, $E_{bb} = -11.21$, and $E_{cc} = 0.30$ MHz and hyperfine interaction constants of $T_{aa} = -183.74$, $T_{bb} = -177.77$, $T_{cc} = 361.51$, and $a_F = 22.8$ MHz. A preliminary structural fit of the rotational constants shows that the bond lengths are close to those of similar compounds and indicates that the angle which measures the deviation of the O atom from the CNC plane is 0° . Details regarding the calculation of the hyperfine interaction and the structural parameters obtained will be discussed.

¹W. H. Kirchoff, J. Mol. Spectrosc. 41, 333 (1972).

*Work supported by NASA Langley

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MG5.

(2:28)

THE MICROWAVE SPECTRA, QUADRUPOLE COUPLING CONSTANTS, AND STRUCTURE OF N-CHLORODIFLUORO-METHANIMINE AND N-BROMODIFLUOROMETHANIMINE

P. GRONER, H. NANAIE, D. DES MARTEAU, AND J. R. DURIG

The microwave spectra of N-chlorodifluoromethanimine (chlorocarbonimidic difluoride), $\text{CF}_2\text{N}^{35}\text{Cl}$ and $\text{CF}_2\text{N}^{37}\text{Cl}$, have been investigated from 18 to 39.5 GHz. The hyperfine structure due to the quadrupole coupling with the chlorine and ^{14}N nuclei has been analyzed for a- and b-type transitions of both isotopic species. From experimental diagonal and off-diagonal quadrupole coupling constants, principal coupling constants of -94.7(1) and -74(1) MHz were calculated for the ^{35}Cl and ^{37}Cl isotopes. A molecular structure compatible with the rotational and quadrupole coupling constants has been determined with $r(\text{N-Cl})$ and $r(\text{C=N})$ having values of 1.700 and 1.254 Å, respectively, and $\angle\text{CNCl} = 116.4(14)^\circ$. The microwave spectra of N-bromodifluoromethanimine (bromocarbonimidic difluoride), $\text{CF}_2\text{N}^{79}\text{Br}$ and $\text{CF}_2\text{N}^{81}\text{Br}$, have also been investigated from 18 to 39.5 GHz. The hyperfine structure due to the quadrupole coupling with the bromine nucleus has been analyzed for the Q-branch transitions of both isotopic species. These data are compared to the corresponding information obtained for the related chlorine compound.

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MG6.

(2:45)

MICROWAVE SPECTRUM AND STRUCTURE OF THE $\text{SO}_2 - \text{H}_2\text{S}$ COMPLEX

R.E. BUMGARNER, D.J. PAULEY AND S.G. KUKOLICH

Rotational transitions for $\text{SO}_2 - \text{H}_2\text{S}$ were measured using a pulsed-beam, Fourier transform microwave spectrometer. Twenty a-dipole and four c-dipole transitions were assigned in the 4-18 GHz range. A, B and C rotational constants were determined to ± 0.1 MHz. An interesting and unusual structure was obtained by fitting these rotational constants. This complex appears to have two $\text{O}\cdots\text{H}$ hydrogen bonds and an $\text{S}\cdots\text{S}$ distance of 3.61 Å. This distance indicates a possible attractive interaction between the sulfur atoms. The $\text{O}\cdots\text{H}$ distance of 2.81 Å is longer than observed for most hydrogen bonds and the complex appears to be rather weakly bound. Data for isotopically substituted species is presently being analyzed.

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THE ROTATIONAL SPECTRUM, STRUCTURE AND DIPOLE MOMENT OF ETHYNYLPHOSPHINE. $H_2PC\equiv CH$

E. A. COHEN, G. A. MCRAE, S. DI STEFANO, R. A. BEAUDET, AND H. GOLDWHITE

The rotational spectra of two isotopic species of ethynylphosphine, $H_2PC\equiv CH$ and $D_2PC\equiv CH$, have been measured in selected regions between 8 and 124 GHz. The rotational constants as well as a complete set of quartic centrifugal distortion constants have been determined for both species. The substitution coordinates of the P hydrogens have been derived. If a reasonable structure is assumed for the $C\equiv C-H$ group, the P-C length and P-C \equiv C angle may be determined from the moments of inertia. The derived structural parameters are $r(P-H)=1.414(5)\text{\AA}$, $r(P-C)=1.774(5)\text{\AA}$, $\angle(P-C\equiv C)=173(2)^\circ$, $\angle(H-P-H)=93.9(5)^\circ$, and $\angle(H-P-C)=96.6(5)^\circ$, with the assumptions $r(C\equiv C)=1.208\text{\AA}$, $r(C-H)=1.058\text{\AA}$, and $\angle(C\equiv C-H)=180.0^\circ$. The $C\equiv C-H$ group is bent away from the hydrogens.

The dipole moment and its orientation have been determined from Stark effect measurements of both species. For $H_2PC\equiv CH$, $\mu_a=0.155(1)\text{D}$, $\mu_c=0.555(1)\text{D}$ and $\mu_t=0.576(1)\text{D}$. For $D_2PC\equiv CH$, $\mu_a=0.138(1)\text{D}$, $\mu_c=0.564(3)\text{D}$ and $\mu_t=0.580(3)\text{D}$. In the normal species the dipole moment makes angles of 53.4° and 70.5° with the P-H and P-C bonds respectively.

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MICROWAVE SPECTRUM OF METHYL DIFLUOROPHOSPHATE

L. RICKUS, H. JUSTNES, J. ZOZOM, C. W. GILLIES, F. J. LOVAS, R. D. SUENRAM, AND T. DIGIUSEPPE

The microwave spectrum of methyl difluorophosphate, $CH_3OP(=O)F_2$, was investigated in the region of 26,500 to 40,000 MHz employing Stark modulation and radiofrequency microwave double resonance (RFMDR) techniques, and in the region of 6000 to 18000 MHz by means of a pulsed beam Fourier transform spectrometer. Under fast scan, low resolution conditions, two ν_a -type prolate rotor band series were observed with B+C values of 4955.5(5) MHz and 4973.4(10) MHz. ν_a - and ν_b -type transitions arising from the 4955.5 band series were found with the pulsed beam spectrometer. However, extensive searches with the Fourier transform system did not reveal the presence of the ν_a -type $J=2 \leftarrow 1$ and $J=3 \leftarrow 2$ lines from the 4973.4 MHz B+C species.

A centrifugal distortion analysis of the ν_a - and ν_b -type transitions obtained in both spectral regions yields the rotational constants (MHz):

$$A = 4568.215(8) \quad R = 2500.728(2) \quad C = 2453.847(2)$$

Efforts to assign the second series by Stark and RFMDR techniques and possible conformational assignments will be discussed.

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MG9.

(3:44)

THE MICROWAVE SPECTRUM OF ARGON-PHOSPHORUS TRIFLUORIDE

K.W. HILLIG, II, J. NATOS, A. SCIOLY AND R.L. KUCZKOWSKI

The argon-PF₃ complex has been prepared in a supersonic expansion of Ar (98%) and PF₃ (2%). A Fourier-transform microwave spectrometer employing a Fabry-Perot cavity was used to assign 28 rotational transitions. The rotational constants (MHz) and distortion constants (kHz) were A = 7332.468(10), B = 1023.055(2), C = 952.564(2), D_J = 3.53(1), D_{JK} = 60.4(1) and d₁ = -0.240(7). The argon atom is 3.953 Å (r_{CP}) from the PF₃ center of mass and r_{CM} makes an angle of 70.3° with the C₃ axis of the PF₃.

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MG10.

(3:56)

HIGH RESOLUTION ROTATIONAL SPECTROSCOPY OF A WEAKLY
BOUND IONIC CLUSTER : Ar.H₃⁺ AND DEUTERATED ISOTOPOMERS

M. BOGEY, H. BOLVIN, C. DEMUYNCK and J.L. DESTOMBES

The first high resolution rotational spectrum of a weakly bound cluster ion is reported. The millimeter and submillimeter wave spectra of Ar.H₃⁺, Ar.D₃⁺, Ar.H₂D⁺ and Ar.DH₂⁺ have been observed in a magnetically confined, liquid nitrogen cooled, negative glow discharge and a molecular structure has been derived from their analysis.

Ar.H₃⁺ is a planar molecule with a C_{2v} symmetry. The Ar atom lies on a symmetry axis of the H₃⁺ quasi-equilateral triangle, 2.38 Å from the H₃⁺ centroid, at a vertex of the triangle.

From the centrifugal distortion coefficient Δ_J, the dissociation energy has been estimated to about 7 - 8 kcal/mole.

Moreover, splitting of some of the lines is strong evidence for tunneling motion.

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MG11.

(4:13)

MICROWAVE SPECTRA OF NOBLE GAS-PYRIDINE COMPLEXES*

T. D. KLOTS, T. EMILSSON, R. S. RUOFF, C. CHUANG, AND H. S. GUTOWSKY

Rotational spectra have been observed for complexes of argon and krypton with pyridine, using a Flygare FTMW spectrometer.¹ Rotational and centrifugal distortion constants have been determined for Ar-pyridine, Ar-[4-D] pyridine and Kr-pyridine, the latter with Kr-82,83,84, and 86. The noble gas atom sits over the pyridine ring in the complex's plane of symmetry. The Ar to pyridine c.m. distance is 3.549 Å, and the line between Ar and the pyridine c.m. makes an angle of 3.40° from the vertical. The results for Ar-[4-D] pyridine show that the Ar is displaced towards the N. The structure of the complex with Kr is very similar. The centrifugal distortion enables estimation of a pseudodiatom force constant and well depth for the dimers. The hyperfine structure from D, ¹⁴N, and ⁸³Kr has been analyzed and will be discussed. A search for the Ar₂-pyridine trimer is in progress. The results will be presented.

*Work supported by NSF and PRF.

¹T. J. Balle and W. H. Flygare, Rev. Sci. Instrum. 52, 33 (1981).

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MG12.

(4:30)

TUNNELING IN DIBORANE-HYDROGEN CHLORIDE DIMERS*

CARL CHUANG, T. D. KLOTS, R. S. RUOFF, T. EMILSSON, AND H. S. GUTOWSKY

K = 0 transitions have been assigned in the microwave rotational spectra for six isotopic variations of the B₂H₆-HCl dimer. The homonuclear dimers, with ¹¹B-¹¹B and ¹⁰B-¹⁰B, have tunneling splittings of several MHz, while the mixed species with ¹⁰B-¹¹B and ¹¹B-¹⁰B show no tunneling. This contrasts with B₂H₆-HF which has a torsionally averaged, linear B-B-F structure with no evidence of tunneling.¹ The line center of the ¹¹B¹¹B-H³⁵Cl J = 3 → 4, K = 0 transition is at 10 186.777 MHz. The splitting due to tunneling is 2.587 MHz, a value which decreases somewhat for both lower and higher J. In the ¹¹B¹¹B-H³⁷Cl species the splitting for J = 3 → 4 decreases to 2.325 MHz while that in ¹⁰B¹⁰B-H³⁵Cl is 4.726 MHz. This indicates that the tunneling motions involve both subunits. Work is in progress to locate the K = ±1 transitions so that accurate rotational constants and the structure can be deduced. The results so far indicate a near linear B-B-Cl configuration.

*Work supported by NSF and PRF.

¹H. S. Gutowsky, T. Emilsson, J. D. Keen, T. D. Klots, and C. Chuang, J. Chem. Phys. 85, 683 (1986).

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MG13.

(4:47)

EXPERIMENTAL SEPARATION OF TORSIONAL AND CHARGE REDISTRIBUTION EFFECTS IN ROTATIONAL SPECTRA OF HCN DIMERS

R. S. RUOFF, T. EMILSSON, C. CHUANG, T. D. KLOTS, AND H. S. GUTOWSKY

We have determined B_0 and D_J for the two ^{13}C monosubstituted dimers of HC^{15}N and the two $\text{DC}^{14}\text{N}/\text{HC}^{15}\text{N}$ dimers. With previous results for several other isotopic species,^{1,2} a full substitution structure has been obtained for $\text{HCN}(1)\text{-HCN}(2)$. It leads to torsional amplitudes θ_1 and θ_2 of 13.6 and 9.3° for the two monomers. A second determination, by fitting B_0 for six isotopic species, gives 13.7 and 8.7°. These values are used to separate torsional and charge redistribution effects upon the hyperfine interactions of D and ^{14}N in the dimers. For ^{14}N , about 40% of the difference in χ_a between HCN monomer and dimer is caused for both N(1) and N(2) by charge redistribution. The analysis will be described, also that for $\chi_a(\text{D})$ and the C-D bond length in the dimer.

*Work supported by NSF and PRF.

¹L. W. Buxton, E. J. Campbell, and W. H. Flygare, Chem. Phys. 56, 399 (1981).²A. J. Fillery-Travis, A. C. Legon, L. C. Willoughby and A. D. Buckingham, Chem. Phys. Letters 102, 126 (1983).

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MG14.

(5:04)

FTMW STUDIES OF HYDROGEN-BONDED TRIMERS*

R. S. RUOFF, T. D. KLOTS, C. CHUANG, T. EMILSSON, AND H. S. GUTOWSKY

Rotational spectra have been observed with a Flygare FTMW spectrometer¹ for a number of hydrogen-bonded trimers, most of which are linear and have the HCN dimer as a subunit. Spectroscopic constants have been determined, usually for several isotopic species of each trimer. Their values are given below for the main species. Symmetries, hydrogen-bond lengths and the separation of torsional and charge redistribution effects on the quadrupolar hyperfine structure of ^{14}N (χ_a) will be discussed.

Trimer	B_0 (MHz)	D_J (Hz)	$\chi_a(\text{N})$ (MHz)	
$(\text{HCN})_3$	469.3073	80	-4.047, -4.251, -4.354	
$(\text{HCN})_2\text{-HF}$	699.204	162	-4.061, -4.091	
$(\text{HCN})_2\text{-HC1}$	467.408	87		
$(\text{HCN})_2\text{-HCF}_3$	305.742	51		
$\text{H}_3\text{N}-(\text{HCN})_2$	675.776	180	-3.298, -4.275, -4.402	
$\text{N}_2-(\text{HCN})_2$	435.573	155		
$\text{OC}-(\text{HCN})_2$	421.142	109	-4.222, -4.361	
OC-HCN-HF	615.573	247		
	<u>B</u>	<u>C</u>	<u>D_J</u>	<u>D_{JK}</u>
$\text{C}_2\text{H}_4-(\text{HCN})_2$	480.592	474.098	128	3 770
$\text{C}_3\text{H}_6-(\text{HCN})_2$	374.472	370.177	62	1 160

*Work supported by NSF and PRF.

¹T. J. Balle and W. H. Flygare, Rev. Sci. Instrum. 52, 33 (1981).

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MH1.

(1:30)

OPTICAL CONSTANTS OF C_4N_2 - AN APPLICATION TO TITAN'S ATMOSPHEREM.A. PERERA-JARMER, R.K. KHANNA

Condensed dicyanoacetylene (C_4N_2) has recently been identified as a constituent of Titan's atmosphere.¹ In order to obtain the abundance of a species, it is necessary to obtain its complex refractive indices.

Infrared spectra of crystalline C_4N_2 were obtained for several film thicknesses. The extinction coefficient, α , and therefore the imaginary refractive index, $k = \alpha / (4\pi\nu)$, were calculated as a function of wavenumber, ν . A Kramers-Kronig analysis was performed to determine the real part of the index of refraction, n , for the entire spectral range.

The results on the optical constants and the calculated abundances of condensed C_4N_2 for Titan's atmosphere will be presented.

¹M.A. Perera-Jarmer, R.K. Khanna, R.E. Samuelson, Bull. Am. Astron. Soc., Vol. 18, No. 3 (1986).

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MH2.

(1:42)

ABSOLUTE INTENSITIES AND COMPLEX REFRACTIVE INDICES OF CRYSTALLINE HC_3N IN THE INFRARED REGIONC.M. HUDSON, R.K. KHANNA

Cyanoacetylene (HC_3N) has been tentatively identified as a constituent of Titan's atmosphere. Absolute infrared intensities of the strong absorption bands of crystalline HC_3N have been obtained in our laboratory. These data have been utilized to calculate the complex refractive indices of crystalline HC_3N in the infrared region. These parameters are of utility in the modeling of Titan's atmosphere.

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MH3.

(1:54)

DIFFERENTIAL REFLECTION SPECTROSCOPY: A DIRECT DETERMINATION OF LONG WAVELENGTH OPTICAL MODE FREQUENCIES IN POLAR CRYSTALS

M. E. THOMAS AND R. I. JOSEPH

To the best of our knowledge, no simple scheme has been proposed for a direct determination of optical mode frequencies from observations of reflectivity, R , without detailed curve fitting. It is our purpose to suggest such a scheme.

We shall work in the wavelength, λ , domain. We propose that the transverse optical wavelengths (λ_{T0}) and Longitudinal optical wavelengths (λ_{L0}) correspond to those points where $dR/d\lambda = 0$ is an extrema, that is where $d^2R/d\lambda^2 = 0$. In particular the λ_{T0} s correspond to points where $d^2R/d\lambda^2 = 0$ and $dR/d\lambda < 0$ whereas the λ_{L0} s correspond to points where $dR/d\lambda = 0$ but $dR/d\lambda > 0$. A simple heuristic argument shows that this method will work to the same extent that Chang's¹ method is valid.

Differential reflection spectra of Al_2O_3 , $MgAl_2O_4$, $Al_{2.3}O_{2.7}N_5$ (ALON) and Y_2O_3 will be presented. In most cases well defined peaks are obtained making the determination of the optical mode frequencies straight forward.

¹I.F. Chang, et.al. Phys. Status Solidi 28, 663 (1968)

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MH4.

(2:06)

INFRARED SPECTROSCOPY OF CO ADSORBED ON SODIUM CHLORIDE SURFACES

H.H. RICHARDSON AND G.E. EWING

The physisorption of CO on sodium chloride surfaces was probed by Fourier Transform Infrared Spectroscopy. Information concerning adsorption and desorption kinetics as well as the critical parameters which govern this reaction, such as binding energy and frequencies for molecule-substrate vibrations, has been obtained for CO adsorbed on NaCl films. These parameters are determined from a family of isotherms in the temperature range between -80K and 100K. Experiments have been extended to single crystal surfaces and a comparison between results on films and single crystal surfaces will be presented.

I. H.H. Richardson, C. Baumann and G.E. Ewing, Surface Science, (in press).

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CRYSTAL VIBRATION OF BETA BARIUM METABORATE AND ITS PHASE TRANSITION
BY RAMAN SCATTERING

GUOZHEN WU, BOGANG TIAN AND XAOJUN LAI

(A) The Raman and i.r. spectra of the newly synthesized second harmonic generating crystal β -barium metaborate in the low temperature phase are presented with a complete assignment of the external and internal vibrational modes. Emphasis is put on the discussion of the site group effect, the isotope effect and the dynamic coupling between the external and the internal motion of the metaborate ring and the barium ion. Force constants are also calculated with the prediction that there is one internal vibrational mode of the metaborate ring at a frequency of 177 cm^{-1} which is of the order of the frequencies of the lattice modes.

(B) The Raman spectra of beta barium metaborate crystal are presented in the temperature range from 25°C to 400°C. The spectra reveal that, as the temperature rises, the frequencies of the internal modes are unaffected. However, those of the lattice modes decrease slightly by about 3 cm^{-1} . Results also show that the phase transition between the low and high temperature phases which are known in the literature occurs over a wide temperature range with no significant changes spectroscopically except the enhancement of the intensity of the translational mode of barium ions at 86 cm^{-1} as the temperature rises. Most intensity enhanced is of E symmetry. The enhancement is most drastic around 217°C and 317°C. It is interpreted that the phase transition is mainly due to the rearrangement of the barium ions in the crystal. As the temperature rises, more barium ions are shifted to the sites of C_3 and D_3 symmetries. The role of the barium ion is also discussed along with its relationship with the second harmonic generating property of the beta barium metaborate crystal.

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MH'1.

(3:00)

TRANSFER AND STORAGE OF VIBRATIONAL ENERGY IN LIQUIDS: COLLISIONAL UP-PUMPING OF CARBON MONOXIDE ON LIQUID ARGON**R. DISSELKAMP AND G.E. EWING**

Isotopically enriched carbon monoxide (88% $^{13}\text{C}^{16}\text{O}$, 12% $^{13}\text{C}^{18}\text{O}$) dissolved in liquid argon was optically pumped to the $v = 1$ level by a cw CO laser. This energy is redistributed by collisional up-pumping to higher vibrational levels. Fluorescence from vibrational levels up to $v = 37$ of the heavier isotope was observed from the steady-state distribution. A discontinuity in the fluorescence at $v = 28$ is observed which happens to be isoenergetic with the excited $a^3\Pi$ electronic state of CO. The $X^1\Sigma + a^3\Pi$ intersystem crossing behavior and reactions which form isotopic carbon dioxide will be discussed.

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MH'2.

(3:17)

TIME-RESOLVED FLUORESCENCE DEPOLARIZATION OF DODCI IN ETHYLENE GLYCOL: EFFECT OF ORIENTATIONAL CORRELATION ON ELECTRONIC EXCITATION TRANSPORT**P. A. ANFINRUD AND W. S. STRUVE**

In an earlier fluorescence depolarization study of singlet excitation transport in glycerol solutions of DODCI [1], physically large discrepancies were observed between experimental fluorescence profiles and profiles calculated from current transport theories [2,3]. Artifacts arising from fluorescence self-absorption, excitation trapping by dye aggregates, and solvent reorganization were ruled out as sources of these discrepancies.

In this work, the study was repeated for DODCI in ethylene glycol, a far less viscous solvent than glycerol. The orientational diffusion of DODCI was characterized in this solvent at low concentration, and its contribution to fluorescence depolarization at higher concentrations was separated from the contribution arising from excitation transport. Analysis of the fluorescence profiles then yields close agreement with transport theories. These results strongly suggest that the discrepancies observed in glycerol are caused by orientational correlation (nonrandomness) in the more viscous solvent.

¹D. E. Hart, P. A. Anfinrud, and W. S. Struve, J. Chem. Phys. **86**, in press.

²D. L. Huber, D. S. Hamilton, and B. Barnett, Phys. Rev. **B16**, 4642 (1977).

³C. R. Gochanour, H. C. Andersen, and M. D. Fayer, J. Chem. Phys. **70**, 4254 (1979).

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MH'3.

(3:29)

INTERNAL ROTATION-VIBRATION COUPLING CONTRIBUTIONS TO VIBRATIONAL LEVEL MIXING IN S_1
p-FLUOROTOLUENE

R.J. LONGFELLOW AND C.S. PARMENTER

A comparison of two spectroscopically and structurally similar molecules, p-difluorobenzene (pDFB) and p-fluorotoluene (pFT), reveals the vibrational level mixing is greatly enhanced in pFT. Parmenter and Stone have suggested that this is due to the methyl rotor levels coupling to vibronic levels of the ring. Evidence for this coupling has been observed in dispersed fluorescence spectra of excited S_1 internal rotation levels in a cold molecular beam. The excitation of specific rotor states provides a test of a recently published¹ mechanism for this internal rotation-vibration coupling. A comparison of these results to selection rules for the mechanism will also be presented.

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1. D.B. Moss, C.S. Parmenter and G.E. Ewing, J. Chem. Phys. 86, 51 (1987).

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MH'4.

(3:46)

DETERMINATION OF THE TORSIONAL POTENTIAL IN GLYOXAL BY ELECTRONIC SPECTROSCOPY

K.W. BUTZ, J.J. JOHNSON, D.J. KRAJNOVICH, AND C.S. PARMENTER

The motion corresponding to internal rotation in glyoxal is a vibrational mode (ν_7) which can be probed by electronic spectroscopy. We have obtained the energy levels of this torsional mode in the ground state trans well corresponding to $\nu_7(\text{trans}) = 0, 1, 2, \dots, 14$ and in the ground state cis well corresponding to $\nu_7(\text{cis}) = 1$ and 2 by electronic SVL fluorescence spectroscopy and by S_1-S_0 excitation spectroscopy in cold molecular beams. These energy levels fit to a Fourier cosine expansion of the torsional potential give an improved picture of the ΔH and barrier to cis \rightarrow trans interconversion.

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MH'5.

(4:03)

THE p-DIFLUOROBENZENE-AR VAN DER WAALS COMPLEX. SPECTROSCOPY, IVR AND VIBRATIONAL PREDISSOCIATION

K.W. BUTZ, H.-K. O, M.-C. SU, AND C.S. PARMENTER

The S_1 p-difluorobenzene-Ar (pDFB-Ar) complex¹ has been characterized by fluorescence excitation spectra and by fluorescence spectra after pumping each of twelve S_1 vibrational levels ranging up to $\epsilon_{vib} = 1250 \text{ cm}^{-1}$. In some cases, additional fluorescence spectra were obtained with initial excitation of the Ar-ring stretch. These spectroscopies constrain the S_0 complex well depth to be $160 < D_0'' \leq 212 \text{ cm}^{-1}$ with the excited state well depth about 30 cm^{-1} greater. The fluorescence spectra variously contain structure from the initially pumped complex level, other complex levels, and the pDFB monomer. This structure shows that vibrational predissociation time scales are generally in the nsec range but vary modestly for different initial modes. Vibrational predissociation is in every case highly selective with respect to formation of "product" vibrational levels in S_1 pDFB monomer. IVR within the S_1 complex occurs from a few of the initial levels and appears to be highly sensitive to the level identity.

1. K.W. Butz, D.L. Catlett, Jr., G.E. Ewing, D.J. Krajnovich and C.S. Parmenter, J. Phys. Chem. 90, 3533 (1986)

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MH'6.

(4:20)

VIBRATIONALLY INELASTIC SCATTERING FROM I_2 AND GLYOXAL IN A NEW CROSSED MOLECULAR BEAM EXPERIMENT

K.W. BUTZ, DU HONG, D. KRAJNOVICH, AND C.S. PARMENTER

A new crossed molecular beam experiment is based on electronic fluorescence spectroscopy after laser pumping of selected ro-vibrational levels in excited states. The spectroscopy provides relative cross sections for single-collision rotationally and vibrationally inelastic scattering to specific final states with close control over collision energies. Experiments that involve collisions of $B^3\Pi_{0+u} I_2$ (initial $v' = 15$ or 25 or 35) and collision partners such as He show all possible Δv changes with the amount of energy transferred approaching the collision energy. The relative cross sections are in fair correspondence to classical trajectory calculations. The total cross sections for vibrationally inelastic scattering is large, being entirely competitive with that for rotationally inelastic scattering. Scattering from several initial levels in S_1 glyoxal also show relatively large cross sections. In this case there is high selectivity among the glyoxal modes that can participate in the energy transfer. Cross sections for excitation of rotations and of the glyoxal torsion (ν_7) depend primarily on ΔE without distinguishing between rotational or vibrational excitation.

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MH'7.

(4:37)

ROTATIONAL AND VIBRATIONAL COLLISIONAL ENERGY TRANSFER IN $^{13}\text{CH}_3\text{F}$ H. EVERITT, R. I. McCORMICK, D. D. SKATRUD, AND F. C. DE LUCIA

We report the results of a detailed study of the rotational-vibrational energy transfer processes in the symmetric top $^{13}\text{CH}_3\text{F}$. This work has been done by observing in real time the relaxation of the nonthermal population placed in $J=5, K=3$ of the ν_3 vibrational state by a Q-switched CO_2 laser. Millimeter and submillimeter wave spectroscopic techniques were used as a sensitive diagnostic probe. Energy transfer processes observed include fast rotational relaxation of velocity subsets within $K=3$, transfer of population to other K states via direct $\Delta K=3n$ processes as well as a "K-swap" mechanism that transcends the selection rules imposed by spin statistics, the transfer of population to the ν_6 and other higher lying vibrational states, and the relaxation of the vibrational population. For the vibrational relaxation, both direct molecule-molecule and wall relaxation were observed. In addition, the wall relaxation channel was shown to require several wall collisions. All of these observations have been fit to a global simulation of the population flow within this system. This model accounts for the observed behavior with a small number of molecular parameters, all of which are physically identifiable.

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Address of McCormick: Department of Physics, United States Military Academy, West Point, NY 10996

Address of Skatrud: Physics Division, Army Research Office, Research Triangle Park, NC 27709

MH'8.

(4:54)

CN $B^2\Sigma^+$ ALIGNMENT FOLLOWING VUV DISSOCIATION OF ICNJ. A. Guest and F. Webster

Dispersed CN $B^2\Sigma^+ \rightarrow X^2\Sigma^+$ photofragment fluorescence polarization anisotropies measured following ICN dissociation at 157.6 nm vary widely and apparently erratically with emission wavelength, and cannot be converted directly to CN B rotational alignments because of spectral congestion. A flexible linear regression technique is used to extract CN $B^2\Sigma^+$ alignments for $v'=0, 1, 2$, and 3. These alignments range from -0.31 to nearly 0.2 and vary smoothly with N' for each v' . A model is presented to estimate partial channel CN B ($v'=0$) product populations, and a discontinuity in the experimental $v'=0$ alignment is considered.

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MH'9.

(5:11)

PHOTOFRAGMENTATION SPECTROSCOPY OF ALKYL NITRITES IN THE $\pi \rightarrow \pi^*$ CHARGE TRANSFER BANDSally S. Hunnicutt and Charles A. Wight

Methyl nitrite and tert-butyl nitrite have been photolyzed in their charge transfer $\pi \rightarrow \pi^*$ bands at 44,400 cm^{-1} . The nascent internal energy distribution of the resulting NO fragment was monitored via 2+2 multiphoton ionization spectroscopy. The NO rotational distribution of both nitrites appeared to be bimodal, with a colder Boltzmann portion overlapped by a high energy tail. The total rotational energy was calculated to be 1050 cm^{-1} . NO was not formed in states higher than $v''=0$.

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Address of Hunnicutt: University of Cincinnati, Department of Chemistry, Cincinnati, Ohio, 45221 (current address). The work was performed at the University of Utah.

TA1.

(8:30)

DEUTERIUM NUCLEAR HYPERFINE SPLITTINGS OF ROTATIONAL TRANSITIONS

S. JANS-BÜRLI AND A. BAUDER

Deuterium quadrupole splittings of rotational transitions have been observed for benzene-d₁, for ortho-, meta-, and para-fluorobenzene-d₁ and for deuterated isothiocyanic acid (DNCS). A gaseous mixture diluted by argon has been expanded through a pulsed supersonic nozzle into an evacuated high Q Fabry-Perot microwave resonator. Highly resolved rotational spectra have been detected with the pulsed excitation and Fourier transform technique. Due to the extremely small dipole moment of benzene-d₁, the molecules have been excited with microwave pulses of up to 10 W. Deuterium quadrupole coupling constants of benzene-d₁ and the three fluorobenzene-d₁ showed little variation.

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TA2.

(8:47)

ISOTOPE EFFECTS IN THE HIGH RESOLUTION INFRARED SPECTRA OF OC-HF

G.T. FRASER AND A.S. PINE

Infrared spectra of OC-HF, O¹³C-HF, and ¹⁸OC-HF have been observed in the vicinity of the HF stretching fundamental using a difference frequency laser spectrometer and a long pathlength thermal equilibrium (T ~ 195 K) White cell. The results on the OC-HF isotopic form extend previous White cell and molecular beam measurements by Kyro *et al.*¹ and Jucks *et al.*². The ν₁ band origins for the complexes; 3844.0294 cm⁻¹ for OC-HF, 3843.7284 cm⁻¹ for O¹³C-HF, and 3843.8731 cm⁻¹ for ¹⁸OC-HF, are all red shifted from the fundamental of uncomplexed HF and do not exhibit a systematic trend with CO stretching or bending frequency. The observed positive ΔB values (B'-B'') are consistent with the increased van der Waals binding in the ν₁=1 excited state. The homogeneous linewidths for the transitions are large (HWHM ~ 180 MHz with roughly equal contributions from pressure broadening and vibrational predissociation) and essentially isotope independent. Local perturbations are observed for OC-HF and ¹⁸OC-HF, but not for O¹³C-HF.

¹ E.K. Kyro, P. Shoja-Chaghervand, K. McMillan, M. Eliades, D. Danzeiser, and J.W. Bevan, *J. Chem. Phys.* **79**, 78 (1983).

² K.W. Jucks and R.E. Miller, *J. Chem. Phys.* (to be published).

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ROTATIONAL SPECTRUM AND STRUCTURE OF H₂CO-HCl

C. W. GILLIES, G. T. FRASER, J. ZOZOM, F. J. LOVAS AND R. D. SUENRAM

Rotational spectra of H₂CO-H³⁵Cl, H₂CO-H³⁷Cl, D₂CO-H³⁵Cl, and D₂CO-H³⁷Cl have been observed using a pulsed nozzle Fourier transform microwave spectrometer. For H₂CO-H³⁵Cl the following spectroscopic constants have been determined (in MHz): B=2687.856(23), C=2527.412(23), Δ_J=0.0105(12), Δ_{JK}=-0.223(10), eQq_{aa}=-41.424(14) and eQq_{bb}=14.106(19). The HCl subunit is bonded to the oxygen of the H₂CO subunit through a non-linear hydrogen bond. For the H₂CO-H³⁵Cl complex, the distance between the centers of masses of the two units is 3.3487 Å giving an O--Cl distance of 3.22 Å. From the quadrupole coupling constant, eQq_{aa}, an effective vibrationally averaged angle between the HCl axis and the a-axis of the complex is determined to be 30.5°. Centrifugal distortion analysis yields estimates of the weak bond stretching force constant and stretching frequency as 0.069(8) mdyn/Å and 85(4) cm⁻¹ respectively. The structural results are compared with the predictions of Buckingham and Fowler¹ from their electrostatic model.

¹A. D. Buckingham and P. W. Fowler, J.Chem.Phys. 79, 6426 (1983).

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ROTATIONAL SPECTRA OF Ar-CH₃OH, Ar-CD₃OH, AND Kr-CH₃OH

R. D. SUENRAM, G. T. FRASER, F. J. LOVAS, J. ZOZOM, and C. W. GILLIES

Microwave spectra of Ar-CH₃OH, Ar-CD₃OH, and Kr-CH₃OH have been obtained using a pulsed nozzle Fourier transform microwave spectrometer. For each of these complexes two torsional states are observed at the ~ 1 K rotational temperature of the expansion. These are the ground state and a metastable excited internal rotor state which correlates to the E internal rotor state of methanol. The a-type ground state spectra are well characterized by the usual asymmetrical top formalism while the excited internal rotor states are complicated by the internal angular momentum. Attempts are presently underway to analyze the excited state spectra. Some preliminary spectroscopic constants for the ground internal rotor state of Ar-CH₃OH complex are (in MHz):

A	25547(15)	Δ _J	0.021887(41)	δ _K	0.342(26)
B	2084.178(52)	Δ _{JK}	0.37189(26)		
C	1928.701(52)	δ _J	0.001622(24)		

The rare gas atom is located approximately perpendicular to the C-O axis. For Ar-CH₃OH the distance between the centers of mass of the two subunits is 3.68 Å and the weak bond stretching force constant is 0.017 mdyn/Å.

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TA5.

(9:33)

ROTATIONAL SPECTRUM AND INTERNAL ROTATION IN CH₃OH-NH₃

G. T. FRASER, F. J. LOVAS, R. D. SUENRAM

The microwave spectrum of the CH₃OH-NH₃ complex has been obtained using a pulsed nozzle Fourier transform microwave spectrometer. The spectrum, which is complicated by the internal rotation of the CH₃ and NH₃ groups, exhibits 5 K=0 states at the ~ 1 K rotational temperature of the expansion. Four of these states are metastable, excited internal rotor states and correlate to E states of free CH₃OH or free NH₃. The observed quadrupole hyperfine patterns are used as a guide in assigning J, K, and torsional quantum numbers to the measured transitions. The quadrupole coupling constant, eQq_{aa}, for the complex is -3.176(7) MHz and B + C is ~ 7375 MHz. The structure of the complex has the OH group of the methanol subunit hydrogen bonded to the nitrogen of the NH₃ subunit. The hydrogen bond length determined for the complex, 2.0 Å, is essentially the same as that found in the related HOH-NH₃ complex, 1.97 Å¹.

¹ P. Herbine and T.R. Dyke, J.Chem.Phys. 83, 3768 (1985).

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TA6.

(9:50)

VIBRATIONAL PREDISSOCIATION SPECTROSCOPY OF HCN CLUSTERS

D.S. ANEX AND G.E. EWING

Vibrational predissociation spectra of HCN clusters formed in a supersonic expansion were obtained in the C-H stretching region. An F-center laser was scanned in the low resolution mode ($\Delta\nu \approx 10$ GHz) while the decrease in molecular beam signal due to recoiling predissociation fragments was monitored using a liquid He cooled bolometer. The C-H stretching frequency is a sensitive probe of cluster size and of monomer position within the cluster. As a result, the evolution of vibrational frequency shifts due to hydrogen bond formation may be followed from small cluster size (dimer, trimer) to large aggregates that exhibit a solid-like absorption feature. The vibrational energy shifts will be discussed with respect to normal mode analysis, electrostatic interactions and ab initio results. Also, the potential of (HCN)_n complexes to provide a model system to explore the development of other properties as clusters grow from isolated molecules into condensed phases will be discussed.

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TA7.

(10:20)

NEGATIVE ION PHOTOELECTRON SPECTROSCOPY OF Rb_n^- , $n=2,3$

K. M. McHugh, J. G. Eaton, G. H. Lee, J. S. Snodgrass, and K. H. Bowen

We have recorded the negative ion photoelectron (photodetachment) spectra of Rb_2^- and Rb_3^- using 2.540 eV photons. Both of these spectra are highly structured, and each exhibits transitions to several electronic states of their corresponding neutrals. The electron affinity of Rb_2 is found to be about 0.5 eV, in agreement with theoretical predictions. The EA of Rb_3 , on the other hand, appears to be about 0.8 eV, and thus deviates from the value expected based on an extrapolation of theoretical predictions for Na_3 and K_3 . The goal in these experiments is not only to map the variation of alkali cluster electron affinities as a function of cluster size, but also to chart the changing electronic states of neutral alkali clusters with size. The hope is that we may eventually be able to start to see the evolution of band structure in these systems.

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TA8.

(10:37)

NEGATIVE ION PHOTOELECTRON SPECTROSCOPY OF: $\text{NO}^-(\text{Ar})_1$, $\text{NO}^-(\text{Kr})_1$, $\text{NO}^-(\text{Xe})_1$, AND N_2O_2^-

C. B. Freidhoff, G. H. Lee, J. T. Snodgrass, and K. H. Bowen

We have recorded the photoelectron (photodetachment) spectra of the gas-phase negative ions: $\text{NO}^-(\text{Ar})_1$, $\text{NO}^-(\text{Kr})_1$, and $\text{NO}^-(\text{Xe})_1$ using 2.409 eV photons, and of N_2O_2^- using both 2.540 eV and 2.707 eV photons. All of these ions were generated in a supersonic expansion ion source with various mixtures of nitric oxide and rare gases. All of the rare gas negative cluster ion spectra exhibit structured spectral patterns which strongly resemble that obtained for free NO^- , but which are shifted to lower electron energies with their individual peaks broadened. Each of these spectra is interpreted in terms of a largely intact NO^- sub-ion which is solvated and stabilized by its rare gas solvent atom. The ion-solvent dissociation energy for a given $\text{NO}^-(\text{Rg})_1$ cluster ion dissociating into NO^- and Rg is given by the energy difference between the origin peak of the free NO^- spectrum and the origin peak of a given $\text{NO}^-(\text{Rg})_1$ spectrum. The values of these shifts were found to be: 0.058 ± 0.011 eV, 0.099 ± 0.018 eV, 0.161 ± 0.024 eV for the argon, krypton, and xenon complexes, respectively. Values for the electron affinities of these complexes were found to be: 0.095 eV, 0.136 eV, and 0.204 eV for the argon, krypton, and xenon complexes, respectively. Both of our photoelectron spectra for N_2O_2^- came at the low electron energy end of our spectral range. The electron affinity of the N_2O_2 species studied here can be given a lower bound of 2.1 eV. Studies by Johnson¹ at higher photon energies indicate the existence of other isomers as well.

¹M. A. Johnson (private communication)

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TA9.

(10:54)

VIBRATIONAL PREDISSOCIATION SPECTROSCOPY OF CLUSTER IONS: INFRARED SPECTRA OF THE CLUSTERS H_n^+ AND $H_3O^+ \cdot (H_2)_m$

M. OKUMURA, L. I. YEH, and Y. T. LEE

The vibrational spectra of the hydrogen cluster ions H_n^+ ($n = 5, 7, 9, 11, 13,$ and 15) and the clusters $H_3O^+ \cdot (H_2)_m$ ($m = 1, 2,$ and 3) have been observed from 3000 to 4200 cm^{-1} , by detecting the laser-induced vibrational predissociation of the clusters trapped in a radio-frequency octopole ion trap.¹ We have observed the H_2 stretching modes near 4000 cm^{-1} of the clusters H_n^+ , with $n = 5, 7, 9, 11, 13,$ and 15 , as well as the "symmetric" H_3^+ stretch in H_5^+ . With the exception of H_5^+ , the frequencies are in good agreement with scaled values predicted by *ab initio* theory. The results are consistent with the theoretical structure of H_2 molecules "solvating" a H_3^+ core, and support the prediction that H_9^+ is a particularly stable species, having a completed inner shell of three H_2 , one at each corner of the H_3^+ . Despite an intensive search of the H_5^+ spectrum at a resolution of 0.1 cm^{-1} , no rotational structure has yet been observed, suggesting that H_5^+ dissociates very rapidly.

We have also obtained vibrational spectra of clusters containing one to three H_2 solvating the hydronium ion H_3O^+ . We have observed all (free and hydrogen-bonded) OH vibrations, as well as the H_2 stretching modes of these clusters. The frequencies are in good agreement with unpublished *ab initio* calculations of Remington and Schaefer. At a laser resolution of 0.5 cm^{-1} , we have observed partially resolved rotational structure in two of the bands of the cluster $H_3O^+ \cdot (H_2)$, the first evidence that rotational information can be obtained from cluster ion predissociation spectroscopy.

¹M. Okumura, L. I. Yeh, and Y. T. Lee, *J. Chem. Phys.* **83**, 3705 (1985).

Present Address of Okumura: Department of Chemistry, The University of Chicago, Chicago, Illinois 60637.

Address of Yeh and Lee: Materials and Molecular Research Division, Lawrence Berkeley Laboratory, and Chemistry Department, University of California, Berkeley, California 94720.

TA10.

(11:11)

INFRARED SPECTRA OF THE HYDRATED HYDRONIUM ION CLUSTERS $H_3O^+ \cdot (H_2O)_m$, $m=1-3$

M. OKUMURA, L. I. YEH, J. D. MYERS, and Y. T. LEE

Vibrational spectra from 2300 to 4000 cm^{-1} of the hydrated hydronium ion in the gas phase have been observed using two new variations of the ion trapping/photodissociation technique. Spectra are obtained by mass-selecting the cluster ion, trapping, exciting the ions with a tunable IR laser, and detecting dissociation products. The new methods have been developed because these clusters are too strongly bound to be dissociated by exciting a single vibrational quantum. In the first experiments, we have observed the vibrational predissociation spectrum of the clusters $H_3O^+ \cdot (H_2O)_m(H_2)$.² Excitation of an OH stretch leads to loss of the H_2 . Because the H_2 binds weakly to the ion, the observed predissociation spectrum provides a low resolution (1 cm^{-1}) spectrum of the cluster $H_3O^+ \cdot (H_2O)_m$. Perturbations induced by the H_2 are observable, and provide additional information. In the second set of experiments, the spectra of the $H_3O^+ \cdot (H_2O)$ clusters are observed by dissociating the clusters themselves. Clusters with OH vibrations excited by a tunable infrared laser are preferentially dissociated (relative to unexcited ions) by multiphoton dissociation (MPD) with a CO_2 laser.

The spectra confirm earlier low resolution (40 cm^{-1}) gas phase spectra observed by Schwarz,¹ and agree with *ab initio* predictions of the vibrational frequencies. Both free and hydrogen-bonded OH stretches have been observed at low resolution (1 cm^{-1}) for $H_3O^+ \cdot (H_2O)_m$, with $m = 1, 2,$ and 3 . Using the two laser MPD approach, rotational structure has also been observed in some bands of $H_3O^+ \cdot (H_2O)$ and $H_3O^+ \cdot (H_2O)_3$ with Doppler-limited linewidths of 0.02 cm^{-1} .

¹H. A. Schwarz, *J. Chem. Phys.* **67**, 5525 (1977).

²M. Okumura, L. I. Yeh, J. D. Myers, and Y. T. Lee, *J. Chem. Phys.* **85**, 3705 (1986).

Present Address of Okumura: Department of Chemistry, The University of Chicago, Chicago, Illinois 60637.

Address of Yeh, Myers, and Lee: Materials and Molecular Research Division, Lawrence Berkeley Laboratory, and Chemistry Department, University of California, Berkeley, California 94720.

TA11.

SOLVATED ALKALI ION CLUSTERS: PRODUCTION AND PRELIMINARY VIBRATIONAL
PREDISSOCIATION SPECTRA

WEN-LONG LIU AND JAMES M. LISY

By combining thermionic alkali ion sources with a supersonic nozzle, abundant solvated alkali ion clusters in the formula $M(X)_n^+$: $M = Na, K, Rb, Cs$ and $X = NH_3, C_2H_4, H_2O, \text{ and } CH_3OH$ ($n = 1$ to 20), have been produced. Individual cluster species are resolved by quadrupole mass spectrometry. Details of the experimental apparatus will be presented.

The principal goal of this study is to characterize the solvation process at the microscopic level. The initial probe of the solvent environment as a function of cluster size uses vibrational predissociation spectroscopy in an analogous manner to neutral cluster studies.¹ The results from preliminary spectroscopic investigations will be presented.

¹D.W. Michael and J.M. Lisy, J. Chem. Phys. 85, 2528 (1986).

Address of Liu and Lisy: Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, IL 61801.

TA12.

AN INVESTIGATION OF THE "SOFT" TORSIONAL MODES OF $(HF)_3$

KIRK D. KOLENBRANDER AND JAMES M. LISY

$(HF)_3$ has been previously shown¹ through the investigation of the H-F stretch vibrational mode to exist in cyclic form in molecular beams. The work reported here marks our effort to extend the investigation of cyclic $(HF)_3$ to the soft modes which display torsional motion of the HF monomer subunits.

A general computational approach has been implemented for the evaluation of the torsional state energies of weakly bonded n-mers. Essentially, this is a large-scale expansion of the n-coupled rotors, but neglects torsional-stretching interactions or coupling with intramolecular vibration. We show how this can be applied to the $(HF)_3$ system, where we have used an idealized, electrostatic surface of Liu and Dykstra².

The results of the theoretical study have been used to direct an experimental investigation of these same modes which is currently underway. Preliminary results of this investigation will be presented.

¹D.W. Michael and J.M. Lisy, J. Chem. Phys. 85, 2528 (1986).

²S.-Y. Liu and C.E. Dykstra, Chem. Phys. 107, 343 (1986).

Address of Kolenbrander and Lisy: School of Chemical Sciences, University of Illinois at Urbana-Champaign, 505 S. Mathews, Urbana, IL 61801.

TA13.

(12:02)

HIGH VIBRATIONAL LEVEL SPECTROSCOPY OF POTASSIUM DIMER

John S. Ozcomert and Patrick L. Jones

The technique of optically pumped supersonic molecular beam lasers is applied to the problem of high vibrational level spectroscopy in the potassium dimer. This method of creating molecular beams of highly excited ground state molecules for scattering or spectroscopy uses the non-equilibrium molecular beam as the gain medium for an optically pumped laser. Downstream of the active region, laser-induced fluorescence on the vibrationally excited molecules is performed. Analysis of the results and the potentials for potassium dimer will be presented and compared with the general trends in other alkali molecules.

Address of Ozcomert and Jones: Department of Chemistry, The Ohio State University, Columbus, Ohio 43210.

TB1.

(8:30)

THE RELATIVE MERITS OF POLARIZING VS AMPLITUDE DIVISION FOURIER TRANSFORM SPECTROSCOPY

H. BUIJS AND C. TRIPP

The BOMEM DA3 Fourier transform spectrometer can now be operated either in the normal amplitude division mode or in the polarization division mode. As described by Dignam and Baker¹ the polarizing interferometer permits direct measurement of differential polarization state absorption and retardation; linear and circular dichroism and their corresponding dispersions.

The polarizing interferometer can also be employed for true optical null dual beam spectroscopy and general single beam spectroscopy as described by Martin and Puplett².

The combination of polarizing interferometry and modern data acquisition and processing techniques appears useful in a number of applications both in low resolution and high resolution spectroscopy.

¹Dignam, M.J., and Baker, M.D. (1981).Appl.Spectroscopy,35,186

²Martin,D.E., and Puplett,E. (1969).Infrared Physics.10,105

Address: Bomem Inc., 625 Rue Marais, Vanier, Quebec, Canada, G1M 2Y2.

TB2.

(8:47)

EXPERIMENTAL RESULTS FROM THE LOS ALAMOS FOURIER TRANSFORM SPECTROMETER

B. PALMER and R. S. McDOWELL

The Los Alamos Fourier transform spectrometer (FTS) is designed for a resolution of 0.0013 cm^{-1} over the spectral region from 200 nm to 15 μm and beyond. The servo accuracy is ~ 1 milli-fringe and data is acquired with an A/D converter having an effective range of 22 bits (1 part in 4 million). It can obtain data at a rate of 25 kHz, or, with the use of a digital filter to increase the S/N ratio, 2-12 kHz. The facility housing the FTS has provision for work with radioactive materials, access to the outside atmosphere and to the sky, and power and cooling facilities to handle a wide variety of laboratory experiments. Areas have been set aside for experimental setups so that more than one experimenter can use the facility at a given time. There is also a computer system for data analysis.

The instrument became operational in its vacuum tank in the Spring of 1987, and we will present and discuss some of the first spectra, demonstrating the wide wavelength coverage and high resolution that the instrument is capable of obtaining. We will also discuss planned experiments and eventual arrangements for outside users of the FTS.

Address: University of California, Los Alamos National Laboratory, Los Alamos, N.M. 87545.

TB3.

(9:04)

LINESHIFT MODULATION FOURIER TRANSFORM SPECTROSCOPY

M. Elhanine, R. Farrenq and G. Guelachvili

The feasibility of selectively recording the line transitions of paramagnetic species using Fourier transform spectroscopy has been demonstrated recently [1]. Essentially the fringe variation producing the interferogram signal is not due to the path difference modulation but to the spectral shift of the lines of interest. In the particular case of paramagnetic species this shift is obtained by applying a magnetic field to the sample. The technique is widely known in laser spectroscopy as 'Laser Magnetic Resonance'. In both FTS and LMR spectroscopies it requires high resolution capabilities.

This paper reports low resolution Zeeman modulation absorption spectra of NO recorded with a Fourier transform interferometer. Only the lines corresponding to transitions between the $\Omega=3/2$ levels are detected. The observed phenomena is essentially understood as due to the variation of the equivalent width of the lines with their splitting by the magnetic field. The absorption process must be in the non linear domain. When this condition is fulfilled, this lineshift modulation has the advantage of being accessible to low resolution techniques. It is likely usable for convenient concentration measurements. Because low resolution runs may be rapidly performed, it may also clearly save time when for instance, the functioning of a source producing unstable species is monitored by a Fourier transform spectrometer.

[1] G. Guelachvili, J. Opt. Soc. Am. B., 3, 1718-1721, (1986)

Laboratoire d'Infrarouge, Associé au CNRS, Bât. 350, Université Paris XI, 91405 ORSAY-Cédex, FRANCE.

TB4.

(9:21)

FUNDAMENTAL LIMITS TO PRECISION IN MEASUREMENT OF PEAK HEIGHT, POSITION, AND WIDTH IN FOURIER TRANSFORM SPECTROSCOPY

A. G. MARSHALL AND L. CHEN

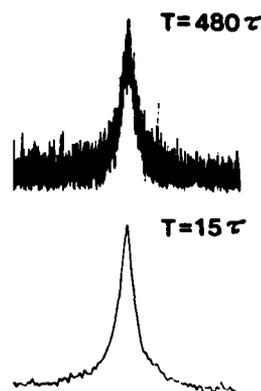
Theoretically, it should be possible to predict the precision, $P(i)$, for multiple determinations of an experimental peak parameter (i = height, width, and position) by least squares fit to a given peak shape from the signal-to-noise ratio (S/N) and number of data points per line width (K) of a single spectrum [1]:

$$P(i) = c(i) \cdot S/N \cdot \sqrt{K}$$

in which $c(i)$ is a line shape-dependent constant [1]. Thus, a sufficiently high digital resolution (i.e., large K) can overcome a poor S/N--see Figure. For Fourier transform spectra, the best precision should thus result from infinite acquisition period ($S/N \rightarrow 0$)!

For FT/NMR and FT/ion cyclotron resonance mass spectrometry, for which noise is independent of the signal strength, we find that the predicted precision falls short of the experimental value by up to an order of magnitude. Possible rationales and prospects will be discussed. We urge optical spectroscopists to test the precision formula, to see whether or not it holds for their experiments. [This work was supported by N.I.H. GM-31683, NSF CHE-8218998, SCEE-SRAP/86-29, and The Ohio State University.]

Figure 1. FT/ICR mass spectra of N_2^+ , for two different acquisition periods, T , in which τ = time-domain damping constant. Top: $S/N = 12.3$; peak position precision = 247. Bottom: $S/N = 63.6$; peak position precision = 216.



L. Chen, C. E. Cottrell, and A. G. Marshall, Chemometrics & Intelligent Lab. Systems 1, 51-58 (1986).

Address: Dept. of Chemistry, The Ohio State University, 120 W. 18th Ave. Columbus, OH 43210

TB5.

(9:33)

NEW HETERODYNE FREQUENCY MEASUREMENTS ON OCS AND FREQUENCY CALIBRATION TABLES BASED ON OCS AND N₂O

A. G. MAKI, and J. S. WELLS

New heterodyne frequency measurements have been made on OCS absorption lines between 1860 and 1915 cm⁻¹. Transitions from the ground state and from low lying vibrational states have been measured. By combining certain heterodyne measurements of hot bands with earlier heterodyne measurements, we obtain accurate calibration data in the 2700 to 3000 cm⁻¹ region. The present heterodyne measurements use a CO laser as a local oscillator (or intermediate frequency standard) and a tunable diode laser locked to the peak of the OCS absorption line. The frequency of the local oscillator is measured against well known CO₂ laser transitions at the same time that the CO-OCS frequency difference is measured.

A summary of frequency calibration data available for OCS and N₂O will be presented. The heterodyne measurements will be compared with some recent FTS measurements from other laboratories as well as from our own laboratory.

Address of Maki: Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, MD 20899.

Address of Wells: Time and Frequency Division, National Bureau of Standards, Boulder, CO 80303.

TB6.

(9:50)

USING A WAVEMETER WITH TUNABLE INFRARED DIODE LASERS

M.D. MARSHALL, H. LEW, N. MARMET, A.R.W. MCKELLAR, and G.W. NICHOLS

We have built an automatic infrared wavemeter¹ based on a fringe-counting Michelson interferometer. It features compact vacuum-tight construction, a vernier technique to ensure integral fringe counts, and the use of an inexpensive home computer (Radio Shack Co-Co 2) board to implement direct automatic read-out of laser wavenumber (cm⁻¹) or wavelength (μm). The design emphasizes compactness and ease of use, and its accuracy is generally limited by diode laser wavefront curvature and alignment effects. For operation in the 5 to 10 μm region, the accuracy is usually about 0.003 cm⁻¹ or better, and this can be improved to about 0.001 cm⁻¹ by a single calibration in a given region to correct for alignment effects. We will discuss some test results obtained with OCS, as well as the problems and advantages encountered in the routine use of this instrument.

¹ H. Lew, N. Marmet, M.D. Marshall, A.R.W. McKellar, and G.W. Nichols, Appl. Phys. B 42, 5 (1987).

Addresses of Marshall, Lew, Marmet, McKellar, and Nichols: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada.

TB7.

(10:07)

NEAR-INFRARED SPECTROSCOPY WITH DFB LASERS

H. SASADA

Semiconductor lasers in the 1.3 to 1.5 μm region are rapidly developed for the demand of optical communication, and a DFB (Distributed Feedback) laser which operates at a single longitudinal mode is available. It is an excellent light source not only for optical communication but for molecular spectroscopy. It has a lot of advantages over Pb-salt diode lasers widely used for infrared spectroscopy: it operates at room temperature, needs no monochromator, and continuously sweeps its frequency over 50 cm⁻¹ without any gaps and jumps. The emitted power is large and smoothly varied against change of injection current and frequency.

Absorption spectra of NH₃ and HCN are recorded from 6460 cm⁻¹ to 6570 cm⁻¹ with two DFB lasers and the molecular constants of some excited vibrational states will be reported.

Address of SASADA: Department of Physics, Faculty of Science and Technology, Keio University, 14-1 Hiyoshi 3-Chome, Kohoku-ku, Yokohama, 223 Japan.

TB8.

(10:35)

QUADRATIC HERMAN-WALLIS FACTORS FOR THE FUNDAMENTALS OF LINEAR MOLECULES

JAMES K. G. WATSON

The effect of vibration-rotation interactions on the intensities of allowed lines of linear molecules can be represented by the Herman-Wallis¹ correction factors

$$F^{PR} = [1 + a_1 m + a_2^{PR} m^2]^2, \quad m = J+1 \text{ (R branch), } -J \text{ (P branch); } F^0 = [1 + a_2^0 J(J+1)]^2.$$

For fundamental bands the a_1 and a_2 coefficients correspond to the terms \tilde{M}_{12} and \tilde{M}_{13} of the effective dipole moment operator^{2,2}. In this work explicit formulas are derived for the a_2 coefficients in the fundamentals of linear molecules. The calculation of these parameters requires up to cubic potential derivatives and quadratic dipole derivatives. A comparison is made between the calculated values for the fundamentals of carbon dioxide and those recently measured by Johns³.

¹ R. Herman and R. F. Wallis, J. Chem. Phys. 23, 637 (1955).

² M. R. Aliev and J. K. G. Watson, in "Molecular Spectroscopy: Modern Research" (ed. K. Narahari Rao), Vol. III (Academic Press, 1985).

³ J. W. C. Johns, paper presented at this symposium.

Address of Watson: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada K1A 0R6.

TB9.

(10:52)

ABSOLUTE INTENSITY MEASUREMENTS OF THE 2.7 μm BANDS OF CO_2 C. M. DEELEY AND J. W. C. JOHNS

Absolute intensities have been measured in the two combination bands, $10^{\circ}1 - 00^{\circ}0$ and $02^{\circ}0 - 00^{\circ}0$, of CO_2 have been measured in the 2.7 μm region. The two other bands have also been measured. Preliminary results indicate that the values of δv , the band intensities, are a little lower than had been thought previously.

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TB10.

(11:04)

ABSOLUTE INTENSITY MEASUREMENTS IN THE ν_2 AND ν_3 FUNDAMENTALS OF CO_2 J. W. C. JOHNS

Absolute intensities have been measured for about 340 lines in the region of the ν_3 fundamental of CO_2 and a rather smaller number of lines in the region of the ν_2 fundamental. The band intensities (in $\text{cm}^{-2}/\text{atm}$ at 300 K) have been found to be 205 and 2219 respectively for ν_2 and ν_3 . Herman-Wallis factors, used to describe the influence of vibration-rotation interaction on the line intensities, have also been determined and are found to agree well with theory.

Some of the precautions taken to ensure accurate measurements will be described.

Address of Johns: Herzberg Institute of Astrophysics, National Research Council Canada, 100 Sussex Drive, Ottawa, Ontario, Canada K1A 0R6.

TB11.

(11:21)

TDL INVESTIGATION OF THE Q-BRANCH OF CO₂ NEAR 720 CM⁻¹

T. HUET, N. LACOME AND A. LEVY

The 14-15 μm region is of particular importance in the remote sensing of atmospheric temperatures. The $10^0 - 01^0$ transition of CO₂ has therefore been investigated in order to determine accurate values of the line intensities and half-widths in the Q-branch.

A double beam TDL mounting was used. Slow scans of the spectra were performed, allowing the simultaneous recording of the line profile along with the fringes of Ge etalon. All measurements were carried out at room temperature for pressures ranging from 5 to 20 Torr in order to avoid excessive overlapping of lines.

Eighteen lines were analyzed from Q(6) to Q(48). The transition moment is found to be equal to 0.1184 D. The obtained line widths exhibit a systematic departure of 10-15 $10^{-3} \text{ cm}^{-1} \text{ atm}^{-1}$ as compared to the averaged values currently observed so far in a great number of CO₂ parallel bands. This might explain some discrepancies in the retrieval of atmospheric temperatures from satellite observations.

Address : Laboratoire d'Infrarouge, associé au CNRS, Bat. 350, Université Paris-Sud,
91405 Orsay Cedex, France.

TB12.

(11:33)

 ν_2 REGION OF CO₂: TEMPERATURE DEPENDENCE OF N₂- AND SELF-BROADENING COEFFICIENTS

T. HUET, C. CHACKERIAN, JR., G. GUELACHVILI, N. LACOME, A. LEVY, AND K. N. RAO

High signal to noise transmission spectra have been obtained of CO₂ under N₂- and self-broadening conditions in the temperature range 300-210 K and pressure range 10-700 torr. Broadening coefficients are reported for the ν_2 and $\nu_2+\nu_1$ vibrational bands.

Address of Huet, Guelachvili, Lacomé, Levy: Laboratoire d'Infrarouge, Batiment 350, Université de Paris sud, 91405 ORSAY cedex, France.

Address of Chackerian: NASA-Ames Research Center, Moffett Field, CA 94035.

Address of Rao: Department of Physics, The Ohio State University, Columbus, OH 43210.

TB13.

(11:50)

Collisional Line Mixing in an N₂-Broadened CO₂ Q BranchL. L. Strow and B. M. Gentry

Rotational collisional narrowing, or line mixing, has been observed in the (11¹⁰,03¹⁰)₁₋₀₀₀ band of CO₂ at 2076 cm⁻¹ using a tunable diode laser spectrometer. Spectra of 1% concentrations of CO₂ in N₂ were recorded at total pressures ranging from 100 to 720 torr. The experimentally determined absorption coefficients are up to 65% lower in the Q-branch wing and 20% larger inside the Q branch than those calculated assuming isolated Lorentz lines. A simple energy gap scaling law is used to determine the off-diagonal relaxation matrix elements from the known pressure-broadening coefficients. The spectra calculated using these matrix elements reproduce the observed absorption coefficients to within several percent. The accuracy of Rosenkranz's first-order theory for the calculation of line mixing will be discussed.

Our observation of line mixing in an N₂-broadened CO₂ Q branch demonstrates that line mixing may be important for a number of problems in atmospheric spectroscopy. The implications of Q-branch mixing for several satellite instruments that employ CO₂ Q branches for remote sounding of atmospheric temperature profiles will be discussed.

Address of Strow: Department of Physics, University of Maryland Baltimore County, Catonsville, Maryland 21228.

Address of Gentry: Code 617, NASA/Goddard Space Flight Center, Greenbelt, Maryland 20771.

TB14.

(12:00)

Collisional Line Mixing in N₂O Q BranchesL. L. Strow and A. S Pine

Rotational collisional narrowing, or line mixing, has been observed in both the $\nu_1+\nu_2$ and $\nu_2+\nu_3$ Q branches of N₂O near 1880 and 2800 cm⁻¹ using a difference-frequency spectrometer and a tunable diode laser spectrometer. Spectra were recorded at pressures ranging from 1 to 740 torr, all self-broadened. The observed pressure-broadened widths of Q(1) through Q(33) in $\nu_1+\nu_2$ agree with those reported by Lacombe et. al.¹ for the P and R branches of the $2\nu_1$, $\nu_1+2\nu_2$, $2\nu_2$, and ν_1 bands to within several percent.

Line-mixing effects are most evident between Q(15) and Q(1) and above the Q-branch head at pressures of 200 torr and greater. Deviations between the observed absorption coefficients and those calculated using the normal isolated Lorentz line model are as large as 50% at 1 atm. A simple energy gap scaling law is used to model the off-diagonal relaxation matrix elements from the observed pressure-broadening coefficients. Spectra calculated from these matrix elements substantially reproduce the experimental data if it is assumed that 1/2 of all collisions place the molecule into ℓ -doubled rotational states that are not accessed by the Q-branch transitions.

¹N. Lacombe, A. Levy, and G. Guelachvili, Appl. Optics. 23, 425 (1984).

Address of Strow: Department of Physics, University of Maryland Baltimore County, Catonsville, Maryland 21228.

Address of Pine: Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Maryland 20899.

TC1.

(8:30)

ABSOLUTE FLUORESCENCE QUANTUM YIELDS OF AZULENE FROM THE S_1 MANIFOLD
SUDHIR. K. KULKARNI, AND JONATHAN. E. KENNY

For the first time, fluorescence from the S_1 to S_0 transition has been observed in a planar supersonic jet. Simultaneous measurements of direct absorption and fluorescence excitation from the S_1 manifold of azulene have been made, and absolute quantum yields calculated. Excited-state lifetimes have been inferred from the primarily homogeneously broadened linewidths, allowing us to obtain approximate nonradiative rate constants for the unusually rapid $S_1 \rightarrow S_0$ internal conversion of levels with 0 to $\sim 1000 \text{ cm}^{-1}$ of excess vibrational energy.

Address of Kulkarni and Kenny: Department of Chemistry, Tufts University, Medford, MA 02155.

TC2.

(8:47)

HYDROGEN BONDING IN GROUND AND EXCITED STATES OF PYRAZINE
TE-YANG LIU, JONATHAN E. KENNY, AND WILLIAM R. MOOMAW

In the complex of pyrazine-hexafluoroisopropanol, the 0_0^0 of the lowest $n\pi^*$ transition is as sharp as that of the parent and is blue-shifted 408 cm^{-1} , with lifetime shorter than 3 ns. This blue shift roughly gives the hydrogen bond energy in the $S_1(n\pi^*)$ of 2740 cm^{-1} . Our interpretation to the short lifetime is that due to the large stabilization of the hydrogen bond, the S_1 is below $T_2(\pi\pi^*)$, which breaks down the coupling between them, resulting in the quenching of the slow component of fluorescence.

Address of Liu and Kenny: Department of Chemistry, Tufts University, Medford, MA 02155

Address of Moomaw: Department of Chemistry, Williams College, Williamstown, MA 02167.

TC3.

(9:04)

FLUORESCENCE QUANTUM YIELDS OF JET-COOLED AZULENES
TIMOTHY M. WOUDEBERG, SUDHIR K. KULKARNI, AND JONATHAN E. KENNY

Simultaneous measurements of absorption and fluorescence in a pulsed planar supersonic jet were used to determine fluorescence quantum yields of several vibronic levels in the S_2 electronic manifolds of azulene, guaiazulene, and 4,6,8-trimethylazulene. The quantum yields at the spectroscopic origins agreed well with those measured in low-temperature matrices, with the alkyl derivatives having smaller quantum yields than the parent hydrocarbon. However, several interesting new results were obtained in the study of higher-lying single vibronic levels. In azulene, mode-specific behavior was more prominent than in previous static gas studies. Vibronic coupling theory was used to estimate radiative rates for the levels excited, allowing us to infer rate constants for internal conversion as a function of excess vibrational energy.

Address of Kulkarni and Kenny: Department of Chemistry, Tufts University, Medford, MA 02155

Address of Woudeberg: Perkin-Elmer Corp., 761 Main Ave, Norwalk, CT 06859.

TC4.

(9:21)

STRUCTURE DEPENDENT COMPETITION BETWEEN MULTIPHOTON ABSORPTION AND INTRAMOLECULAR ENERGY REDISTRIBUTION IN ORGANOMOLYBDENUM COMPOUNDS: STATE SELECTIVE PRODUCTION OF MOLYBDENUM ATOMS

BRIAN SAMORISKI AND J. CHAIKEN

We have measured one color multiphoton dissociation/ionization (MPD/MPI) spectra for a series of arene molybdenum tricarbonyls. These experiments measure the relative timescales of multiphoton excitation, intramolecular energy redistribution (IER) and unimolecular dissociation under collision free conditions.

Our organometallic MPD/MPI experiments involve focusing a tunable UV-visible laser pulse into a bulk gas sample and recording the total ion yield as a function of laser photon wavenumber. The directly observable spectral features reflect the distribution of metal atom states which is produced by the various dissociation processes that are simultaneously occurring. By studying a series of organometallic molecules whose structures were chosen to give systematic variation of intramolecular couplings and state densities and thus IER rates/paths, we strive to discover how the structure of a particular molecule determines the distribution of metal atom states formed when the ligands are removed by MPD.

We concentrate on the production of ground state metal atoms by MPD from the organo-molybdenum precursors. From our spectra, an even-parity 7S_3 Rydberg series of molybdenum was identified. Members of the analogous $^7D_{1,2,3,4,5}$ series can also be observed. Both of these series have the molybdenum atom ground state as the lower state in each transition. As such, their visibility is a direct indication of the extent of production and ionization of ground state molybdenum atoms by MPD of the parent molecule.

As our results from the study of organochromium compounds suggest, ground state atom production is favored when the ligands are strongly bound to the metal atom and when the ligands have structures that induce the existence of low frequency vibrational modes. Both of these factors tend to facilitate the transfer of internal energy from the metal atom to the ligands.

Address: Department of Chemistry, Syracuse University, Syracuse, New York, 13244-1200.

TC5.

(9:38)

GAS PHASE ELECTRONIC SPECTROSCOPY OF ARENE CHROMIUM TRICARBONYLS: DIRECT DISSOCIATION VS. PREDISSOCIATION IN THE LOWEST ENERGY EXCITED ELECTRONIC STATE

DAN ROONEY AND J. CHAIKEN

We have measured the first gas phase electronic absorption spectra of $(\eta_6\text{-C}_6\text{H}_6)\text{Cr}(\text{CO})_3$, $(\eta_6\text{-C}_6\text{H}_5\text{Cl})\text{Cr}(\text{CO})_3$, and $(\eta_6\text{-C}_6\text{H}_5\text{CH}_3)\text{Cr}(\text{CO})_3$ at low resolution, 200 cm^{-1} . These spectra show intense ($92,000\text{ liter/mole-cm}$) absorption features extending into the vacuum ultraviolet indicating the existence of at least five different electronic states with energies below 61000 cm^{-1} . Our low resolution data suggest that only one of those states shifts appreciably with arene substitution. We compare these results with solution phase spectra and other data. At higher resolution, 40 cm^{-1} , our data suggest that the onset of detectable absorption is lower in energy for $(\eta_6\text{-C}_6\text{H}_6)\text{Cr}(\text{CO})_3$ than both $(\eta_6\text{-C}_6\text{H}_5\text{Cl})\text{Cr}(\text{CO})_3$, and $(\eta_6\text{-C}_6\text{H}_5\text{CH}_3)\text{Cr}(\text{CO})_3$. The vibronic envelope of this transition suggests significant structural deformation occurs with the electronic transition. The deformation may be correlated with the well known photolability of the CO ligands. We speculate that the lowest energy excited electronic state of the ACl is dissociative with respect to the CO ligands. We also demonstrate that there is a significant increase in the number of low frequency vibrations upon mono-substitution of the benzene ring. We discuss these new data in the light of our earlier multiphoton spectroscopy results on these molecules.

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SYMPOSIUM ON MOLECULAR SPECTROSCOPY (42ND) HELD IN
COLUMBUS OHIO ON JUNE 15-19 1987(U) OHIO STATE UNIV
COLUMBUS DEPT OF PHYSICS K N RAO 19 JUN 87

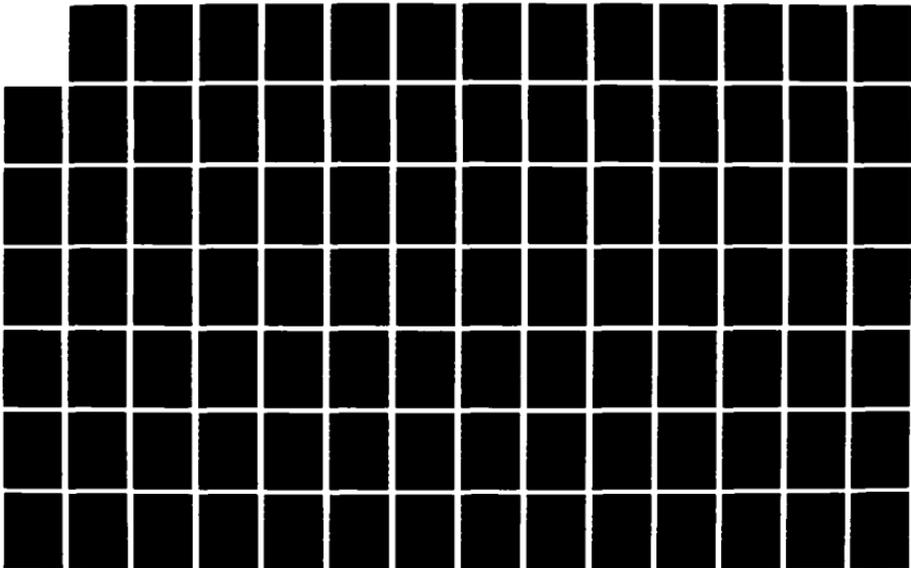
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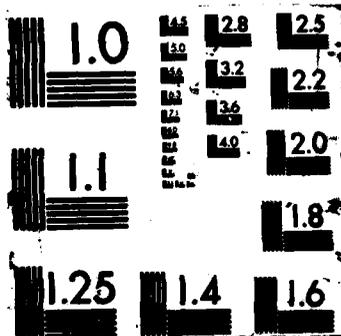
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TC6.

(9:55)

ELECTRONIC TRANSITION MOMENT DIRECTIONS OF THE ADENINE CHROMOPHORE

Leigh B. Clark

The electronic spectrum of the adenine chromophore has been reinvestigated using single crystal polarized reflection spectroscopy. The original assignments of the low energy absorption region (260 nm in solution) were made over twenty years ago and since then have been the basis for almost all the numerous spectroscopic interpretations and calculations of the electronic properties of polynucleotides containing the adenine residue. New spectra obtained from crystals of 9-methyladenine and 6-methylaminopurine suggest that the original assignments are incorrect. The present data lead to an interpretation in which two overlapped transitions of comparable intensity are to be found in the low energy spectral region. The transition moment directions of the slightly lower energy component is about -6° (positive angles are measured counterclockwise from the central C_4-C_5 bond). The second and somewhat more intense band is polarized at $\sim +48^\circ$. Some comments regarding the higher energy bands (~ 200 nm) as well as the mixing effects owed to intermolecular interactions in the crystal will be presented.

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TC7.

(10:25)

HYDROGEN BONDED CLUSTERS OF TRYPTOPHAN AND RELATED COMPOUNDS

L. A. PETEANU, L. A. PHILIPS, Y. D. PARK, and D. H. LEVY

The spectra of various hydrogen bonded clusters of the amino acid tryptophan and related molecules have been obtained using both fluorescence excitation and resonantly enhanced two photon ionization spectroscopies. In the jet cooled spectra of tryptophan, tryptamine, and indole propionic acid multiple distinct conformations of each of these molecules can be identified. In several cases, the preferred conformation of the molecule appears to be different in the cluster than in the isolated species. As a result, these clusters exhibit solvent induced shifts which are anomalous when compared to those observed for the common chromophore indole.

The effect of complexation on other properties of the electronic states of these molecules will be discussed as well.

James Franck Institute, Univ. of Chicago, Chicago, Illinois 60637

TC8.

(10:42)

SPECTROSCOPY OF JET-COOLED p-DICHLOROBENZENE AND p-DICHLOROBENZENE - ARGON VAN DER WAALS COMPLEX

W. D. SANDS AND R. MOORE

Fluorescence excitation spectra have been obtained for p-dichlorobenzene in a pulsed supersonic expansion in He, Ar, and dilute Ar/He mixtures. Prominent in the spectra are vibronic features which have not been observed in previous spectra obtained under bulb conditions. Van der Waals features appear 30 $1/cm$ and 60 $1/cm$ to the red of bare molecule features and are identified as p-dichlorobenzene - argon van der Waals complexes containing one and two argon atoms, respectively.

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TC9.

(10:59)

CHEMILUMINESCENCE FROM LASER-HEATED SOLID AND GASEOUS TETRAMETHYLDIOXETANE

M. A. TOLBERT, M. J. ROSSI, and D. L. HUESTIS

We have been investigating the spectrally and temporally resolved emissions from the decomposition of laser-heated solid and gaseous tetramethyl-1,2-dioxetane.

In the solid-phase studies, a collection of small crystals was held between salt windows, through which passed a $0.5-1.5 \text{ J/cm}^2$ $1 \mu\text{s}$ pulse from a CO_2 laser. After an incubation period of $2-12 \mu\text{s}$ a sharp spike of visible emission occurs, lasting $1-5 \mu\text{s}$. After a further delay of about $30 \mu\text{s}$, emission resumes until about $500 \mu\text{s}$. The sharp spike and the delayed emission yield the same spectrum, peaking around 410 nm , with a FWHM of $30-50 \text{ nm}$. The spectrum, which exhibits reproducible structure, is in the position expected for singlet acetone, but is substantially narrower.

In the gas-phase studies, decomposition is sensitized by an infrared absorbing gas (CH_2F or SF_6). The decomposition temperature is varied by adjusting either the laser fluence or the pressures of sensitizing and inert buffer gas (N_2). Decomposition temperatures are estimated to be in the range $550 \text{ K} - 850 \text{ K}$. The luminescence accompanying high temperature decomposition is shown to be identical to acetone fluorescence. The measured fluorescence quantum yield at low temperature, 550 K , is similar to that reported previously for fluorescence from electronically excited acetone, 0.001 , and decreases with increasing temperature.

The combination of gas- and solid-phase decomposition studies indicate that the narrow, structured spectrum observed for the solid is not entirely due to high temperature. The high density of the solid sample may be the factor that leads to the unusual emission spectrum observed.

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TC10.

(11:16)

PHOTOINDUCED ABSORPTION IN EMERALDINE*

J.M. GINDER, M.G. ROE, P.E. WIGEN, A.J. EPSTEIN, M. ANGELOPOULOS, and A.G. MacDIARMID

We report the photoinduced absorption spectrum of the emeraldine base form (EB) of polyaniline, a polymer consisting of phenyl and quinoid rings in a ratio of 3:1 linked by amine or imine nitrogen atoms. When pumped by laser photons of energy $2.0-2.7 \text{ eV}$, EB exhibits a photoinduced bleaching band which peaks at 1.8 eV , as well as two correlated photoinduced absorption bands which peak at $\sim 1.3 \text{ eV}$ and 3.0 eV . Laser power and chopping frequency dependences of the 1.3 eV and 3.0 eV photoinduced absorption bands are nearly identical and differ significantly from those of the 1.8 eV photoinduced bleaching band. The results are compared to a model of photoexcitation of a 2 eV molecular exciton band¹ and formation of positive and negative polarons. We will also discuss the photoinduced absorption spectrum of electrically conducting protonated emeraldine.

*This work supported in part by the Defense Advanced Research Projects Agency through a grant monitored by the U.S. Office of Naval Research.

¹C.B. Duke, E.M. Conwell, and A. Paton, Chem. Phys. Lett 131, 82 (1986)

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TC11.

(11:33)

INTRACONFIGURATIONAL ABSORPTION AND VISIBLE REGION ABSORPTION SPECTROSCOPY OF ReCl_6^{2-} IN VARIOUS $(\text{NR}_4)_2\text{SnCl}_6$ HOST CRYSTALS

S. C. LEE, R. K. YOO, B. A. KOZIKOWSKI, AND T. A. KEIDERLING

Low temperature absorption spectra for Re^{4+} , a d^3 system, in various $(\text{NR}_4)_2\text{SnCl}_6$ ($\text{R} = \text{CH}_3, \text{C}_2\text{H}_5, \text{C}_3\text{H}_7$) host crystals indicate effects of reduced host symmetry and origin shifts. In the $\text{N}(\text{C}_2\text{H}_5)_4^+$ and $\text{N}(\text{C}_3\text{H}_7)_4^+$ containing host crystals, a significant splitting was found that correlated to two substitutional sites with paralleling vibronic patterns. For ReCl_6^{2-} in $(\text{NR}_4)_2\text{SnCl}_6$ ($\text{R} = \text{H}, \text{CH}_3, \text{C}_2\text{H}_5, \text{C}_3\text{H}_7$), several new transitions located from 16000 to 20000 cm^{-1} were found using absorption and excitation spectroscopy, which cannot be assigned to intra-configurational transitions of ReCl_6^{2-} . These may be due to either impurity or interconfigurational transitions. Discussion of these unassignable transitions will be presented.

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TC12.

(11:45)

ELECTRONIC SPECTROSCOPY AND ENERGY TRANSFER PATHWAYS FOR MATRIX ISOLATED I_2

WAFAA FAWZY, M. A. P. MACLER, J.P. NICOLAI, AND M.C. HEAVEN

The electronic spectroscopy of I_2 , isolated in a solid Ar matrix, has been studied using time and wavelength resolved fluorescence excitation techniques.

Low concentration matrices (I_2 : Ar, 1:1000), excited at wavelengths of 532nm or longer, showed only the A-X emission system. Polarization measurements and laser excitation spectra showed that the A state was populated via the $\text{A} \leftarrow \text{X}$ and $^1\pi(1_u) \leftarrow \text{X}$ transitions.

At an I_2 :Ar ratio of 1:600 the $\text{I}^2\text{P}_{1/2} \rightarrow \text{I}^2\text{P}_{3/2}$ emission was observed, in conjunction with the $\text{I}_2 \text{A} \rightarrow \text{X}$ bands. Energy transfer from I_2 (A) was found to be the mechanism by which the atoms were electronically excited.

A vibronic progression, similar to that of the I_2 A-X bands, but shifted to slightly longer wavelengths, was apparent at an I_2 :Ar ratio of 1:300. The lifetime of the emission was extremely long (20ms). Most probably, this red-shifted emission originated from $\text{I}_2(\text{A})$ molecules which were perturbed by other nearby I_2 molecules. A mechanism which accounts for the unexpectedly long lifetime is proposed.

Work supported by AFOSR under grant 85-0210

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TD1.

(8:30)

FTIR ISOTOPIC STUDY OF THE C_2H_3 VINYL RADICAL IN AN ARGON MATRIXRICHARD A. SHEPHERD AND W.R.M. GRAHAM

The C_2H_3 vinyl radical, which was first observed spectroscopically by ESR¹ in matrices, has been found to be one of the products of the vacuum UV photolysis of acetylene trapped in argon at 10 K,² and may also be formed from ethylene. The results of an FTIR investigation of the mid-infrared spectrum of C_2H_3 , using deuterium and carbon-13 isotopic substitution will be discussed, and compared with the predictions of recent *ab initio* calculations³.

¹E.L. Cochran, F.J. Adrian and V.A. Bowers, J. Chem. Phys. **40**, 213 (1964).

²R.A. Shepherd and W.R.M. Graham, J. Chem. Phys., to be published March 1.

³M.N. Paddon-Row and J.A. Pople, J. Phys. Chem. **89**, 2906 (1985).

Address: Department of Physics, Texas Christian University, Fort Worth, TX 76129.

TD2.

(8:47)

VIBRATIONAL AND ELECTRONIC SPECTRA OF THE PRODUCTS OF THE H + HCN REACTION TRAPPED IN SOLID ARGON¹MARILYN E. JACOX

When H atoms produced by photolysis or by a microwave discharge react with HCN and the products are trapped in solid argon at 14 K, several infrared absorptions attributable to species of formula CH_2N appear, as do prominent absorptions of HNC. Filtered mercury-arc photolysis studies have established two different photodecomposition thresholds for the CH_2N species, and isotopic substitution studies are consistent with the identification of H_2CN and with the presence of at least one of the HCNH rotamers. Ultraviolet absorption studies have confirmed the previous assignment of several diffuse bands to H_2CN and have extended the band system for this species to higher frequencies.

¹ Supported in part by the U. S. Army Research Office.

Address: Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, Md. 20899.

TD3.

(9:04)

INFRARED SPECTRA OF GUEST MOLECULES IN CRYSTALLINE CLATHRATE HYDRATE FILMS

J. Paul Devlin and Fouad Fleyfel

The guest molecules in a clathrate hydrate are isolated in well-defined cages. Such systems were difficult to study spectroscopically prior to the demonstration that crystalline films of the clathrate hydrates of polar molecules can be readily deposited from the vapor phase^{1,2}. Recently, as part of a study of the mechanism of the growth of ice-like crystals at low temperatures, infrared spectra of several caged molecules have been measured. The spectra are marked by evidence of dynamical coupling between neighbor guest molecules, Evans holes (i.e., Fano antiresonances) caused by the interaction of guest and host vibrational states, and sharp variations with temperature that reflect the orientational dynamics of the engaged molecules.

¹J. E. Bertie and J. P. Devlin, *J. Chem. Phys.*, **78**, 6340 (1983).

²H. H. Richardson, P. J. Wooldridge and J. P. Devlin, *J. Chem. Phys.*, **83**, 4387 (1985)

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TD4.

(9:21)

THE USE OF ISOLATED ISOTOPOMER SPECTRA IN PROBING THE DEFECT STRUCTURE OF ICE

Paul J. Wooldridge and J. Paul Devlin

Proton transport in hydrogen bonded systems is of importance because of its role in many fundamental processes, e.g., in biological systems. Our ability to form H₂O ice containing D₂O molecules which have not undergone isotopic exchange and to monitor isotopic scrambling spectroscopically has made ice a model system for the exploration of the molecular-level details of proton transport. The electrical and mechanical properties of ice have long been described in terms of the migration of orientational defects and protons along the H-bonded network, assuming no interaction between the defects. It will be shown that, particularly at low temperatures, the mobile proton concentration can be affected by shallow proton traps. The presence and energetics of these shallow traps are revealed by the FT-IR spectra of ice samples subjected to ionizing radiation at low temperatures, and subsequently warmed. This paper will focus on results for uv-irradiated ice samples.

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TD5.

(9:38)

Ag₇ CLUSTER: PENTAGONAL BIPYRAMID

S. B. H. BACH, D. G. GARLAND, R. J. VAN ZEE AND W. WELTNER, JR.

The analysis of a well-resolved electron-spin-resonance (ESR) spectrum of a silver cluster trapped in solid neon at 4°K has established it as Ag₇. ¹⁰⁹Ag hyperfine structure shows that the single electron spin is interacting strongly with two equivalent (axial) Ag nuclei and weakly with five equivalent (equatorial) Ag nuclei. It has D_{5h} symmetry and a ²A₂⁺ ground state. These properties are analogous to its Group IA alkali-metal counterparts.

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Address of Garland: City University of New York, The City College, New York, NY 10031.

TD6.

(9:55)

GROUND STATE OF THE C_6 MOLECULE

R. J. VAN ZEE, R. F. FERRANTE, K. J. ZERINGUE, AND W. WELTNER, JR.

Pure carbon molecules have been trapped in neon and argon matrices at 4°K from the vapor over thermal- or laser-heated graphite or from the microwave discharge of triacetylene in argon. Linear triplet C_4 has previously been identified.¹ Corresponding signals attributed to a linear C_6 molecule in a $^3\Sigma$ state, probably the ground state, are also observed. ^{13}C nuclear hyperfine structure again supports a cumulene-type bonding. The zero-field-splitting parameter was found to be $|D| = 0.363 \text{ cm}^{-1}$ (in neon), about 50% larger than that of C_4 . These results will be discussed relative to recent ab initio calculations.^{2,3}

¹ W. R. M. Graham, K. I. Dismuke, and W. Weltner, Jr., *Astrophys. J.* **204**, 301 (1976).

² K. Raghovachari, R. A. Whiteside, and J. A. Pople, *J. Chem. Phys.* **85**, 6623 (1986).

³ D. W. Ewing (private communication).

Address of Van Zee and Weltner: Department of Chemistry, University of Florida, Gainesville, FL 32611

Address of Ferrante: Department of Chemistry, Wake Forest University, P.O. Box 7486, Winston-Salem, NC 27109

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TD7.

(10:25)

 C_nO MOLECULES

R. J. VAN ZEE AND W. WELTNER, JR.

Simple theory indicates that linear C_nO molecules with n even should have triplet ground states (e.g., C_2O).¹ Those with n odd are expected to be singlets. (Although well-studied,² the experimental ground electronic state of C_3O is not known.) We report here the electron-spin-resonance (ESR) spectra at 4° K of C_4O and possibly C_6O formed from the reactions of CO with carbon molecules. ^{13}C nuclear hyperfine splittings and spin densities are in approximate accord with INDO calculations.

¹ C. Devillers and D. A. Ramsay, *Can. J. Phys.* **49**, 2839 (1971).

² R. D. Brown, *Int. Rev. Phys. Chem.* **5**, 101 (1986); R. D. Brown and E. H. N. Rice, *J. Am. Chem. Soc.* **106**, 6475 (1984); T. B. Tang, H. Inokuchi, S. Saito, C. Yamada, and E. Hirota, *Chem. Phys. Lett.* **116**, 83 (1985).

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TD8.

(10:37)

THE SEARCH FOR PYRIDYNE; MATRIX ISOLATION OF 2,3- AND 3,4-PYRIDINEDICARBOXYLIC ANHYDRIDE AND THEIR PHOTOLYSIS PRODUCTS

H.-H. NAM and G. E. LEROI

FTIR spectra of pyridine-2,3-dicarboxylic anhydride (2,3-PDA) and pyridine-3,4-dicarboxylic anhydride (3,4-PDA) isolated in argon and nitrogen matrices at 15° K have been obtained. Mild photolysis ($\lambda \geq 340$ nm) of modest duration ($t < 100$ min) readily produces CO and CO₂ fragment absorption, plus bands of -C=C- character due to transient species. Since neither terminal -C=N nor -C=C-H frequencies are present, we believe that the intermediates are cyclic in nature; perhaps pyridyne. (Corresponding experiments with phthalic anhydride yield benzyne.¹) Additional photolysis of the matrix isolated samples, however, produces new decomposition products including HCN and diacetylene.

The vibrational spectra of the transient intermediates from 2,3-PDA and 3,4-PDA are quite different in their frequencies and intensities, which suggests that the photolysis products from the two precursors are different in nature. The experimental results will be presented, and interpreted in terms of normal coordinate analyses and considerations of the interactions between the nonbonding electrons of the nitrogen atom and the sp² orbitals of neighboring dehydrogenated carbon atoms.

¹H.-H. Nam and G. E. Leroi, Spectrochim. Acta 41A, 67 (1985); J. Mol. Structure (1987), in press.

Address of Nam and Leroi: Department of Chemistry, Michigan State University, East Lansing, Michigan, 48824.

TD9.

(10:54)

MATRIX ISOLATION SPECTROSCOPY FOR VIBRATIONAL ASSIGNMENTS AND GROUP FREQUENCY DETERMINATIONS

D. PRESSER AND R. J. JAKOBSEN

The matrix isolation spectra of a group of hydrocarbons and polar substituted hydrocarbons indicate that the narrower infrared lines produced by this technique will be exceedingly useful for the determination of functional groups and structural aspects of the hydrocarbon moiety. With the aid of the matrix isolation spectra various types of both methyl and methylene groups can be differentiated in the CH stretching region and thus group frequencies for hydrocarbon components can be determined. Thus, for example, various types of methylene vibrations can be identified and are seemingly strongly influenced by the nature of neighboring groups.

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TD10.

(11:11)

OPTICAL AND ESR SPECTROSCOPY OF MATRIX-ISOLATED ETHYLNITRENE

Robert F. Ferrante, Susan L. Erickson, and Brian M. Peek

The ethylnitrene radical $\text{CH}_3\text{CH}_2\text{N}$ has been produced by the interaction of gaseous ethylazide with metastable N_2 or Ar generated in a microwave discharge, and has been trapped in N_2 and Ar matrices at 10 K. The UV absorption spectrum in solid nitrogen consists of a series of eleven bands beginning at 335 nm with an average vibrational interval of 320 cm^{-1} . Intensity alternations suggest that two different vibrations are excited in the transition, probably a C-C-N bend corresponding to the observed spacing and a C-N stretch with vibrational frequency near 650 cm^{-1} . The ESR spectrum at 8300 G indicates that ethylnitrene has a triplet ground state with zero-field splitting parameters $D = 1.67\text{ cm}^{-1}$ and $E = 0.0033\text{ cm}^{-1}$ in a nitrogen matrix. The hyperfine splittings differ slightly in the x and y lines and have the average values of 16.0 G for N and 30.6 G for the methylene H. The spectral features associated with ethylnitrene were not observed through direct photolysis of the parent ethylazide either during or after deposition. The new optical data confirms previous speculation and expands the assignment of the UV spectrum of ethylnitrene; the high D value indicated by the ESR signals lends support to the suggestion that earlier assignments of the ESR spectrum of methylnitrene, CH_3N , are incorrect.

¹T. Franken, D. Perner and M. W. Bosnali, Z. Naturforsch. Teil A25, 151 (1970).
²R. F. Ferrante, J. Chem. Phys. 86, 25 (1987).

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Address of Peek: Department of Chemistry, University of North Carolina-Chapel Hill, Chapel Hill, NC 27514

TD11.

(11:28)

MAGNETIC CIRCULAR DICHROISM OF CYCLOOCTATETRAENYL MONOANIONS ISOLATED IN ARGON MATRICES

C. Samet, J. Lurito, L. Andrews and P. N. Schatz

The conformation and electronic structure of cyclooctatetraene (COT) and its anions have been of interest for many years. COT has a nonplanar tub structure (D_{2d}) and is nonaromatic. The dianion (COT^{2-}) is almost certainly planar, aromatic, and of D_{8h} symmetry. The situation is less clear with respect to the monoanion (COT^-).

We have measured the magnetic circular dichroism (MCD) of COT^- isolated in Ar matrices by codepositing COT and alkali metal atoms. Bands are observed at about 340 and 300 nm. The former shows a remarkably well resolved series of vibronic A terms. The MCD is temperature independent, strongly supporting the view that the ground state structure of COT^- is consistent with an orbitally degenerate planar configuration subject to a dynamic Jahn-Teller Effect in the b_{1g} in-plane C-C stretching vibration. The lack of MCD temperature dependence allows us to place a lower limit on the strength of the Jahn-Teller coupling.

¹A. D. McLachlan and L. C. Snyder, J. Chem. Phys. 36, 1159 (1962).

Address: Department of Chemistry, University of Virginia, Charlottesville, VA 22901.

TE6.

(4:26)

GAS CORRELATION SPECTROSCOPY OF THE STRATOSPHERE: THE HALOGEN OCCULTATION EXPERIMENT (HALOE)

D. Chris Benner, S. Roland Drayson and James M. Russell III

Since diatomic molecules have relatively few vibration-rotation transitions of significance in the stratosphere, broad band radiometer channels are not an effective means of measuring concentrations of these gases. A gas correlation spectrometer, however, in measuring the correlation between the stratospheric spectrum and the spectrum of a gas in a cell within the spectrometer can effectively pick out the gas of interest. Using the sun as a source and viewing in the occultation mode from Earth orbit, this type of spectrometer has been incorporated into the Halogen Occultation Experiment (HALOE) which will be on the Upper Atmosphere Research Satellite, presently scheduled for launch in 1991. Spectroscopic line parameters have been used to predict the signals that will be seen. The technique is quite sensitive and will provide useful mixing ratio profiles for HF, HCl, NO and CH₄. The sensitivity, however, extends to chance correlations with the spectrum of other gases present in the atmosphere. Spectroscopic parameters required to interpret the data will be reviewed and a list of those not yet sufficiently well known will be presented.

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Address of Russell: Atmospheric Sciences Division, MS401B, NASA Langley Research Center, Hampton, Virginia 23665-5225.

TE7.

(4:38)

STRATOSPHERIC NO_x GAS DISTRIBUTIONS FROM BALLOON-BORNE THERMAL EMISSION SPECTRA

W. A. SHAFFER, M. M. ABBAS, J. C. BRASUNAS, A. GOLDMAN, L. W. HERATH, J. R. HERMAN, V. G. KUNDE, S. T. MASSIE, W. C. MAGUIRE

High spectral resolution thermal emission spectra of the Earth's stratosphere have been analyzed to retrieve stratospheric thermal structure and the mixing ratio profiles of several minor constituents in the NO_x family. The retrieval techniques include line-by-line spectral calculations with an onion-peeling inversion scheme. The retrieved profiles are compared to other observations and a 1-D photochemical model.

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Address of Massie: National Center for Atmospheric Research, P. O. Box 3000, Boulder, Colorado 80307.

TES.

(4:50)

LOWER STRATOSPHERIC TRACE CONSTITUENTS FROM A BALLOON-BORNE CRYOGENIC INTERFEROMETER

W. C. MAGUIRE, M. M. ABBAS, J. C. BRASUNAS, A. GOLDMAN, L. W. HERATH, J. R. HERMAN,
V. G. KUNDE, S. T. MASSIE, W. A. SHAFFER

The infrared emission from minor constituents in the lower stratosphere has been measured using a balloon-borne cryogenic Fourier spectrometer. A liquid-nitrogen cooled interferometer spectrometer with liquid-helium cooled Si:Ga detectors has recorded selected portions of the thermal emission spectrum from 650-2000 cm^{-1} with an apodized resolution 0.03 cm^{-1} . Species identified to date include CO_2 , O_3 , H_2O , CH_4 , HNO_3 , N_2O , NO_2 , NO , ClONO_2 , CCl_3F , and CF_2Cl_2 . A tentative identification of N_2O_5 in the 1230 - 1270 cm^{-1} region has been made.

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Address of Herath and Shaffer: Science Systems and Applications, Inc., Seabrook, Maryland 20706.

Address of Massie: National Center for Atmospheric Research, P. O. Box 3000, Boulder, Colorado 80307.

FORBIDDEN ROTATION TRANSITIONS BETWEEN NUCLEAR SPIN MODIFICATIONS IN POLY-ATOMIC MOLECULES BY NUCLEAR SPIN-ROTATION INTERACTIONS

MAN-CHOR CHAN, K. LALITA SARKAR, and TAKESHI OKA

The nuclear spin-rotation interaction Hamiltonian of polyatomic molecules with different symmetries has been derived with respect to the molecule-fixed axes. Terms diagonal in the basis set $|IJFM_F\rangle$ cause nuclear hyperfine structure whereas the off-diagonal ones give rise to the conversion between different nuclear spin states. The basic difference between them is the symmetry upon permuting the spin coordinates of identical nuclei. Based on Wigner's idea on the stability of ortho- and para- hydrogen,¹ a group theoretical method is developed to discriminate the diagonal terms from the off-diagonal ones. We use an extended group in which pure nuclear permutation operations are added to the usual molecular symmetry group. The diagonal terms are totally symmetric to these added operations while the non-diagonal terms are not. Van Vleck's reverse angular momentum method² has been applied to evaluate the off-diagonal matrix elements. We estimate the order of magnitude of the conversion rate³ due to this interaction and discuss some experimental observations.

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THE ANOMALOUS $k=3$ SPLITTINGS OF PH_3 IN THE ν_2 STATE OBSERVED BY RADIOFREQUENCY-INFRARED DOUBLE-RESONANCE

YIT-TSONG CHEN and TAKESHI OKA

We have observed the $k=3$ splittings in the ν_2 state of PH_3 using radiofrequency-infrared double-resonance. The microwave sidebands on CO_2 laser lines were used as the infrared radiation source. The observed splittings together with those earlier reported by Carlotti *et al.*¹ do not agree with the simple $\frac{(J+3)!}{(J-3)!}$ formula, contrary to the similar splittings in the ground state reported by Klemperer and his colleagues.² A more pronounced anomaly has been reported for the $k=6$ and $k=9$ doublings in the $3\nu_2$ and $4\nu_2$ states of PH_3 .³ We explain the anomaly for the ν_2 state by taking into account the Coriolis interactions between ν_2 $k=3$ levels and various ν_4 $|k-\ell|=3n$ levels. The results explain this anomaly well. We have obtained the following splitting parameters for various doublings:

$$\Delta_{(\nu_2, k=3, \ell=0)} = 357(40) \text{ Hz}$$

$$\Delta_{(\nu_4, k=2, \ell=-1)} = 594(70) \text{ kHz}$$

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TF3.

(2:04)

OBSERVATION OF SMALL SPLITTINGS IN THE VIBRATION-ROTATION SPECTRUM OF PF₅

JOHN ERVE, YIT-TSONG CHEN and TAKESHI OKA

We have used the microwave modulation sidebands CO₂ laser source for sub-Doppler spectroscopy of PF₅ in the 10 μm region,^{1,2} where a great number of spectral lines have been observed corresponding to the fundamental and many hot bands of the ν₃ transition. Under high resolution (Δν ~ 50 kHz) many of the spectral lines for the fundamental band, as well as various hot bands, are split by about 500kHz ~ 1MHz. For most cases the two components of the split lines have about equal intensity. The relation of the observed splitting with the possible pseudorotation of PF₅³ is being investigated.

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TF4.

(2:21)

INFRARED MICROWAVE SIDEBAND LASER SPECTROSCOPY IN THE CO LASER REGION¹

SHIN-CHU HSU, GOTTFRIED MAGERL, AND R. H. SCHWENDEMAN

By using a CdTe electrooptic modulator with broad-band antireflection coatings on the ends, an infrared-microwave sideband laser spectrometer has been assembled for operation in the CO laser region. Except for the higher frequency of the infrared radiation, the operation of the spectrometer is very similar to that of our systems in the CO₂ or N₂O laser regions.² The laser is frequency-stabilized and the microwave frequency is stepped by a computer across the X-band (8-12.4 GHz) or the P-band (12.4-18 GHz). Modulation of the spectrometer signal is achieved by chopping the microwave radiation with a PIN diode. The sidebands are split into sample and reference beams and the amplitude of the reference beam controls the sideband power by controlling the attenuation of the PIN diode during the "on" portion of its cycle. Although the CO laser power is lower than that of our CO₂ lasers, the efficiency of the sideband generation is greater at the higher infrared frequency, so the sideband powers in the two frequency regions are comparable. Currently, the CO laser is frequency-stabilized at the top of the gain curve, which limits the reproducibility of the frequency to ±10 MHz. The results of spectroscopic measurements of N₂O, H₂CO, and HCOOH will be described.

¹This work was partially supported by the National Science Foundation.

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TF5.

(2:38)

INFRARED MICROWAVE DOUBLE RESONANCE WITH A SIDEBAND LASER SPECTROMETER¹DEAN B. PETERSON AND R. H. SCHWENDEMAN

A cylindrical cavity sample cell with ends that transmit 80% of the incident infrared radiation has been constructed for the purpose of carrying out infrared microwave double resonance experiments with high-power microwave pumping radiation and a tunable low-power infrared source. The length of the cavity and the microwave injection port are tunable and the measured Q 's are ~5000. The microwave pumping source is an 8-12 or 12-18 GHz backward-wave oscillator that is amplified to as much as 20 W by means of a traveling wave tube amplifier. The ends of the cell are high-transparency fine mesh metal screens covered by NaCl windows. The path length is ~0.3 m. The infrared source is an infrared microwave sideband laser operating in either the 6 μm or 10 μm region.

The purpose of the high-power pumping is to create a Rabi splitting of the pumped transition that is comparable to the Doppler width, so that the modulation of the infrared absorption caused by switching the microwave power has a magnitude that is a significant fraction of the ordinary infrared absorption. The results of experiments with CH_3OH , CF_3I , and NH_3 will be described.

¹This work was partially supported by the National Science Foundation.

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TF6.

(2:55)

EXPERIMENTAL DETERMINATION OF ELECTRIC FIELDS IN THE POSITIVE COLUMN OF A GLOW DISCHARGE

M. B. RADUNSKY AND R. J. SAYKALLY

Measurement of the absolute Doppler shifts of ions in the positive column of a glow discharge allows the measurement of the plasma electric field responsible for the shift. The $A^2\Pi_u + X^2\Sigma_g^+$ (7,3) band of N_2^+ has been observed by velocity modulation laser spectroscopy and used as a probe of He/ N_2 plasmas. By driving the discharge with a pulse instead of with the conventional sine wave, only one direction of current flow is observed, allowing measurement of the Doppler shift in ion transition frequencies caused by the electric field of the plasma. Fields have been measured as a function of pressure from 1-9 Torr. Values of the electric field range from 3 to 10 V/cm.

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TF7.

(3:20)

EFFICIENCY AND LINewidth IMPROVEMENTS IN A GRAZING INCIDENCE DYE LASER USING AN INTRACAVITY LENS AND SPHERICAL END MIRROR

R. S. Smith and L. F. DiMauro

A modified simple cavity design for the grazing incidence dye laser is presented. Diffraction losses are reduced by the addition of an intracavity lens and 100% reflecting spherical end mirror. The resulting concentric resonator design allows conversion efficiencies of 15% to be achieved. In addition, linewidth reductions of 25-40% over the conventional cavity are obtained, and the effects of the lens design with and without a spherical end mirror are discussed. Linewidth, efficiency, and relative power measurements for the conventional and modified dye laser cavities are compared.

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TF8.

(3:32)

Diode Laser Spectroscopy of a $^3\Pi\text{CO}$

P.B. Davies and P.A. Martin

The absorption spectrum of metastable $^3\Pi\text{CO}$ has been measured in the infrared using a diode laser. The molecule was generated in an air cooled a.c. discharge and signals were detected using concentration modulation (2f detection). Most of the lines can be assigned to the fundamental band ($\Omega=0,1,2$) based on predictions from optical spectroscopy.¹ Lambda doubling splittings in the $\Omega=1$ and 2 manifolds are in good agreement with molecular beam r.f.² and microwave³ results when available. The much larger $\Omega=0$ lambda doublings are easily resolved in the diode laser spectra and provide information on the doubling in this sub-state of the molecule which is not available from rf or microwave results.

-
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TF9.

(3:44)

LASER INDUCED FLUORESCENCE OF CO^+ AND THE $\text{CO } a^3\Pi_1$ STATE PRODUCED BY 2+1 MULTIPHOTON ABSORPTION IN A SUPERSONIC JET

M. Anselment, L. F. DiMauro, and T. A. Miller

We report the first successful demonstration of the production of copious amounts, 10^8 ions/cc, of small molecular ions in a jet expansion via resonantly enhanced multiphoton ionization. The study involves the 2+1 multiphoton ionization via the $B^1\Sigma^+$ state of jet cooled CO molecules. Sufficient downstream densities are achieved to perform rotationally resolved LIF spectroscopy on both the $X^2\Pi \rightarrow A^2\Sigma$ transition of CO^+ and the triplet third positive group of CO. The consequences of experimental conditions on the branching ratio of the products are discussed.

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TF10.

(3:56)

INFRARED SPECTRUM OF THE FO_2 RADICAL

A.R.W. McKellar, J.B. Burkholder, A. Sinha, and C.J. Howard

FO_2 has previously been observed by infrared and ESR techniques in low temperature matrices, but the first gas-phase spectroscopy was reported only recently by Yamada and Hirota¹ who studied the ν_3 band at 579 cm^{-1} using a tunable diode laser spectrometer. We have now recorded and analyzed the ν_1 , $2\nu_1$, $2\nu_3$, $\nu_2+\nu_3$, and $\nu_2+2\nu_3$ bands as well as the previously studied ν_3 fundamental. The experiments were performed in Boulder using a high-resolution (0.0026 cm^{-1}) Bomem FTS and a fast-flow long-path absorption cell; FO_2 was produced using the reaction $\text{F} + \text{O}_2 + \text{M} \rightarrow \text{FO}_2 + \text{M}$. The most interesting aspect of the analysis is the region of the ν_1 fundamental: it turns out that ν_1 (1487 cm^{-1}) is very strongly perturbed by $\nu_2+2\nu_3$ (1496 cm^{-1}) through both Coriolis and homogeneous (Fermi-type) interactions. In contrast, the other bands ν_3 , $\nu_2+\nu_3$ (940 cm^{-1}), $2\nu_3$ (1142 cm^{-1}) were found to be unperturbed. $2\nu_1$ (2948 cm^{-1}) is apparently subject to a number of smaller perturbations, but it could be approximately analyzed without including them. Our work yields an extensive set of molecular parameters for FO_2 , including approximate spin-rotation constants for the states involved. Now only the ν_2 fundamental ($\approx 370 \text{ cm}^{-1}$?) remains unobserved at high resolution.

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TF11.

(4:13)

DIODE LASER SPECTROSCOPY OF THE ν_2 BAND OF THE CD_3 RADICAL*
 J. M. FRYE AND T. J. SEARS

The ν_2 band of the CD_3 radical was observed by diode laser spectroscopy, and subsequent analysis yielded the center frequency and rotational constants for both the ground and $\nu_2 = 1$ states. Radicals were generated by excimer laser photolysis of a slow-flowing CD_3I/He mixture, and spectra were observed after multiple reflection of the diode laser in a White cell configuration. Spectra were recorded using a Boxcar averager, and analysis of the time dependence of the radical concentration will also be presented.

* This research was carried out at Brookhaven National Laboratory under contract DE-AC02-76CH00016 with the U. S. Department of Energy and supported by its Division of Chemical Sciences, Office of Basic Energy Sciences.

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TF12.

(4:25)

NEW VIBRATIONAL BANDS FROM THE $\Pi(010)$ STATE OF THE CCH RADICAL IN THE
 GROUND ELECTRONIC STATE

H. KANAMORI and E. HIROTA

We have recently observed two vibrational hot bands from the $\Pi(010)$ of the ground electronic state of the CCH ($\tilde{X}^2\Sigma^+$) radical by using IR diode laser kinetic spectroscopy.

One band was observed in 1720 cm^{-1} region and was assigned to the $\Pi(011)-\Pi(010)$ transition. Combined with a previous result on the $\Pi(011)-\Pi(000)$ band¹⁾, the ν_2 fundamental frequency was determined for the first time to be $370.1537(15)\text{ cm}^{-1}$. This value is in good agreement with an estimate using the 1-type doubling constant²⁾.

The other band was observed in 1790 cm^{-1} region and the upper state is tentatively assigned to the $\Pi(07^10)$ state from the ν_2 frequency above mentioned.

The vibrational term values, other molecular constants, and the intensity of spectra suggest that the $\tilde{A}^2\Pi$ state perturbs strongly vibrational states of the ground electronic state.

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TF13.

(4:37)

DETERMINATION OF THE MOLECULAR STRUCTURE OF SEVERAL CARBO-CATIONS VIA THE "COULOMB EXPLOSION" TECHNIQUE

LESLIE H. TACK, AUREL FAIBIS, ELLIOT P. KANTER, ZEEV VAGER

Several important carbo-cations such as $C_2H_3^{+1}$ and CH_5^+ have been studied by this radically new technique which obtains direct three-dimensional images of small molecules.

Protonated acetylene has been a molecule of extreme interest because of the possibility of it assuming nonclassical "bridged" and classical "nonbridged" configurations. Our data is consistent with having the proton in the bridged position; the spatial geometry obtained is in quite reasonable agreement with ab initio^{2,3} calculations.

This work supported by the U. S. Department of Energy, Office of Basic Energy Sciences, under Contract W-31-109-ENG-38.

¹E. P. Kanter, Z. Vager, G. Both, and D. Zajman, *J. Chem. Phys.* **85**, 7487 (1986).

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³J. Pople, private communication.

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TF14.

(4:49)

STRUCTURAL DETERMINATIONS OF MOLECULAR IONS BY DIRECT THREE-DIMENSIONAL IMAGING: THE "COULOMB EXPLOSION" EXPERIMENT

A. FAIBIS, L. M. TACK, E. P. KANTER, Z. VAGER

When molecular ions are accelerated to high velocities (0.03c) and passed through extremely thin (50 Å) Formvar targets their valence electrons are stripped off, initiating molecular dissociation on a time scale much shorter (10^{-17}) than vibrational and rotational motion. The individual atoms from the explosion event are detected in coincidence via a novel detector¹ that measures their relative momenta. This information can be uniquely related to the structure of the molecule. The "Coulomb explosion" technique has been used to determine the structure of several carbo-cations e.g.,² ($C_2H_3^{+3}$ and CH_5^+) and represents a powerful new technique for investigating the structure and vibrational motions of molecular ions.

This work supported by the U. S. Department of Energy, Office of Basic Energy Sciences, under Contract W-31-109-ENG-38.

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TF15.

(5:01)

STEREOCHEMICAL INFORMATION ON CH_3^+ AND NH_3^+ DERIVED USING THE COULOMB EXPLOSION TECHNIQUE
AUREL FAIBIS, ELLIOT P. KANTER, LESLEY M. TACK, AND BRUCE J. ZABRANSKY

Structure parameters for CH_3^+ and NH_3^+ molecular ions are extracted from Coulomb-explosion measurements utilizing 4.5-MeV ion beams. A typical experiment determines the relative velocities acquired by the atomic fragments as the molecular ion dissociates. The relative positions of the constituent nuclei, at the moment the dissociation starts, determine the total kinetic energy of the system and the way it is distributed among the atomic fragments. We are in the process of accumulating this type of information for several small molecular ions (total mass smaller than 50 a.m.u.) and have already succeeded to produce information not available through classical methods^(1,2). The CH_3^+ and NH_3^+ ions data reveal structure parameters of these ions as well as correlations between the different internal degrees of freedom.

(1) Z. Vager et al., Phys. Rev. Lett. 57 (1986), p. 2793.

(2) E. P. Kanter et al., J. Chem. Phys. 85 (12), 1986, p. 7487.

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TG1.

(1:30)

HIGH RESOLUTION FOURIER TRANSFORM EMISSION SPECTROSCOPY OF XeH

M. Douay, S.A. Rogers and P.F. Bernath

Electronic transitions of XeH were recorded in the infrared with the Fourier transform spectrometer associated with the McMath Solar Telescope at Kitt Peak.

XeH was made in a nickel hollow cathode discharge lamp with 100 mTorr of Xe and 2.2 Torr of H₂. The high-resolution Fourier transform emission spectrum of a $2\Sigma^+-2\Pi$ transition near 4400 cm⁻¹ was observed and analysed. The molecular constants were obtained for these two states. Other transitions were observed from 2900-3800 cm⁻¹ and 4600-5000 cm⁻¹.

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TG2.

(1:47)

HIGH RESOLUTION VIBRATION-ROTATION EMISSION SPECTRA OF XeH⁺ AND CHS.A. ROGERS, C.R. BRAZIER AND P.F. BERNATH

The infrared spectra of the $X^2\Pi$ state of CH and the $X^1\Sigma^+$ state of XeH⁺ were observed with the McMath Fourier transform spectrometer at Kitt Peak. The 1-0, 2-1, and 3-2 vibration-rotation bands of CH were detected in a microwave discharge of CH₄ in He. The XeH⁺ molecule was made in a nickel hollow cathode discharge lamp containing 2.2 Torr of H₂ and 0.1 Torr of Xe. Molecular constants for ¹³²XeH⁺ include $r_e = 1.602813(6)$ Å, $\omega_e = 226.9674(11)$ cm⁻¹ and $\omega_e x_e = 41.32830(34)$ cm⁻¹.

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TG3.

(2:04)

THE ELECTRONIC STRUCTURE OF GAS PHASE MnH

T.D. VARBERG, J.A. GRAY, AND R.W. FIELD

Sub-Doppler intermodulated fluorescence excitation spectra of the MnH and MnD $A^7\Pi-X^7\Sigma^+$ system reveal hyperfine splittings due to both ^{55}Mn and H (or D). For MnH, a typical low-J $N^+=J'-3, N^-=J''-3$ transition is split into 12 strong hyperfine components: a six component Landé pattern (overall width of ~4 GHz) due to the Mn $I = 5/2$ spin, each component of which is doubled (~210 MHz splitting) by the H $I = 1/2$ spin. The ~210 MHz Fermi contact hyperfine splitting requires nearly a full unpaired electron spin on the hydrogen atom. This seems incompatible with the standard bonding picture for MnH and with the matrix ENDOR spectrum¹.

In order to obtain sub-Doppler spectra of transitions involving J' or $N^+=0$ or 1 levels, for which $\Delta F \neq J'-N^+$ hyperfine transitions will be strong and definitively assignable, the existing rotational analyses² have been extended and corrected. Of the 147 possible rotational branches, Nevin² identified 47 and we have added 19 additional branches. Perturbations in either $A^7\Pi$ or $X^7\Sigma^+$ could provide linkages with expected low-lying $^5\Sigma$ and $^5\Delta$ states, but most of the previously identified MnH perturbations are either due to isolated line misassignments or to rapid evolution from case 'a' to 'b' in the $A^7\Pi$ state.

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TG4.

(2:21)

A NEW SPUTTER SOURCE AND ITS APPLICATION TO THE NiH SPECTRUM

MINGGUANG LI, JEFFREY A. GRAY, AND ROBERT W. FIELD

A long path-length (20 cm), multipass (40x), magnetically confined, sputter source has been designed for laser spectroscopic studies of metal hydride, halide, and oxide diatomic molecules. The source consists of a cylindrical cathode of the metal to be vaporized and 10 sequential anodes (resistively and inductively stabilized). An axial 1-2 kG magnetic field confines the Ar^+ glow discharge and increases the sputtering efficiency 3-10-fold and allows stable operation of the device at pressures as low as 50 mTorr. Laser beams propagate directly through the discharge region where the MX molecules are generated. The 20 cm absorption length may be multiplied by at least 40x by an internal mirror White cell multipass arrangement. The new source is superior to the single anode sputter sources used previously in studies of NiH in providing higher molecule number density, 400x longer absorption length, >5x lower operating pressure, and improved discharge stability. It is well suited to studies of refractory metal containing molecules in which the signal is carried by the transmitted laser beam (direct absorption, magnetic rotation, polarization, transient nutation, and homodyne spectroscopies) rather than laser excited fluorescence. Magnetic rotation and absorption spectra of the weak NiH $\Omega = 3/2, v = 1 + X^2\Delta_{5/2}, v = 0$ band and sub-Doppler polarization spectra of the ~30x stronger NiH $B^2\Delta_{5/2}, v = 1 + X^2\Delta_{5/2}, v = 0$ band have been recorded. The capabilities of this source are still being evaluated, but it appears to be more sensitive by $>10^3$ than Broida oven and single anode sputter sources.

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TG5.

(2:32)

THE GREEN BANDS OF CaO: OODR SPECTROSCOPY AND ELECTRONIC STRUCTURE MODEL

DAVID P. BALDWIN, ROBERT W. FIELD, AND J. NORMAN

The CaO Green and Orange Systems are so complex that their attribution to CaO rather than a polyatomic species was in doubt until recently. Excluding all $1\Sigma^+$ states, the electronic structure of CaO may be understood as Ca^+O^- where the Ca^+ structure ($X\sigma, A\pi, B\sigma$ Ca^+ centered orbitals) is well represented by a ligand field model for the Ca-monohalides¹ and an O^- p-hole (σ^{-1} or π^{-1}). All prominent features of the CaO Orange system have been assigned as transitions between five $A\pi\pi^{-1}$ upper states and two $X\sigma\pi^{-1}$ lower states ($a^3\Pi, A^1\Pi$). The model predicts that the Green System will consist of $B\sigma\pi^{-1} 1,^3\Pi_i - X\sigma\pi^{-1} 1,^3\Pi_i$ transitions analogous to the Green CaF $B^2\Sigma^+ - X^2\Sigma^+$ system.

Laser excitation-resolved fluorescence spectroscopy has confirmed the predicted assignments of the upper and lower states of the CaO Green System. Rotation-vibration analysis of this exceedingly congested system requires a sub-Doppler Optical Optical Double Resonance (OODR) scheme linked via a common lower level in order to select a single J, e/f, Ω component. Preliminary measurements show T_0 and B_0 values for the $B\sigma\pi^{-1} 1\Pi$ state of 26 348 cm^{-1} and 0.353(4) cm^{-1} . This newly discovered 1Π state lies only 435 cm^{-1} above and has a B_0 -value 0.033 cm^{-1} (i.e. 9%) smaller than the known $B^1\Pi$ state. This is in accord with the $A\sigma\pi^{-1}$ configuration of $B^1\Pi$ and provides further evidence for the almost perfect separation of the CaO electronic spectrum into π^{-1} and σ^{-1} sub-manifolds.

S.F. Rice, H. Martin, and R.W. Field, J. Chem. Phys. 82, 5023 (1985).

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TG6.

(2:55)

THE LOW LYING STATES OF SAMARIUM OXIDE

C. LINTON, GUO BUJIN, R.S. RANA AND J.A. GRAY

The spectroscopy of SmO is being investigated as part of a continuing study into the properties and electronic structure of the rare earth oxides. By using laser induced fluorescence and combining the results of resolved fluorescence and high resolution excitation spectra with the sub-Doppler Zeeman patterns obtained in a magnetic field we have established an energy level scheme linking together eleven low lying electronic states and provided conclusive Ω assignments for most of the states. The ground state is determined to be a $\Omega = 0$ state.

The results will be discussed in terms of detailed Ligand Field Theory calculations which have predicted the energies of all the low lying states. The analysis of large Ω doubling in the $\Omega = 1$ states will be explained in terms of the interaction with neighboring $\Omega = 0$ states. The results of this analysis serve as a very useful test of the calculated eigenfunctions for these states.

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TG7.

(3:25)

Vibrational assignment for the $A^2\Pi-X^2\Sigma$ band system of the SiN radical: The 0-0 band of ^{29}SiN and ^{30}SiN

Chikashi Yamada, Satoshi Yamamoto, Shuji Saito, and Eizi Hirota

The vibrational assignment for the A-X system of the SiN radical¹ was reexamined by observing the spectra in the 5- μm region of ^{29}SiN and ^{30}SiN in natural abundance. The original assignment of Mulliken for the A state was found to be correct, rather than the one currently accepted; the 5- μm spectrum was assigned to the 0-0 band of the A-X system. The vibrational and isotopic variations observed for the Λ -type doubling and spin orbit interaction constants of the A state and for the spin-rotation interaction constants of the X state were explained by treating the electronic matrix elements of the spin-orbit interaction and of the orbital angular momentum between A/X, B/A and D/X states as parameters.

1 Chikashi Yamada and Eizi Hirota, J. Chem. Phys. 82, 2547 (1985).

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TG8.

(3:42)

HIGH RESOLUTION LASER SPECTROSCOPY OF NIOBIUM NITRIDE

Y. AZUMA, J.A.BARRY, M.J.P.LYNE, J.O.SCHRODER AND A.J.MERER

The laser induced fluorescence spectrum of gas phase niobium nitride (NbN) in the region 5700 Å to 6300 Å has been recorded with Doppler limited resolution, and also with sub-Doppler resolution by the intermodulated fluorescence technique for selected regions.

The spectrum includes two triplet systems, the $3\Phi-3\Delta$ and the $3\Pi-3\Delta$. Both systems show very impressive hyperfine splittings due to the interaction between the 9/2 Nb nuclear spin and a metal-centered unpaired electron. For the $3\Pi-3\Delta$ system, it has been found that the middle $3\Pi_1-3\Delta_2$ sub-band is shifted from its regular middle position to the lowest position, presumably due to an interaction between the $3\Pi_1$ state and another close lying electronic state. The assignment of the electronic states was aided by the study of hyperfine splitting patterns and also by relative intensities of rotational lines obtained with the wavelength resolved fluorescence technique. Wavelength resolved fluorescence has also shown the existence of other low lying states and the possibility that the real electronic ground state lies still below the 3Δ state.

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TG9.

(3:55)

THE FIRST NEGATIVE BAND SYSTEM OF $^{15}\text{N}_2^+$

S. PADDI REDDY AND C. V. V. PRASAD

The emission spectrum of the first negative ($B^2\Sigma_u^+ - X^2\Sigma_g^+$) bands of the nitrogen-15 ion, $^{15}\text{N}_2^+$, excited in a hollow cathode discharge tube of a special design has been investigated in the spectral region 3570 - 5170 Å. The rotational structure of thirteen bands involving $v' = 0, 1$ and 2 and $v'' = 0$ to 5 were photographed in the 2nd and 3rd orders of 2 m and 3.4 m grating spectrographs. Spin-splitting of the rotational levels has been measured for several of the observed bands. Perturbations are observed in the $v = 0$ level of the B state. At the time of preparing this abstract the rotational analysis of seven bands has been completed and that of the rest of the bands is in progress. The results of the analysis of all the thirteen bands will be presented.

¹Research supported in part by NSERC Grant No. A-2440.

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TG10.

(4:16)

ABSOLUTE ABSORPTION CROSS SECTION MEASUREMENTS OF OZONE AND THE TEMPERATURE DEPENDENCE

K. YOSHINO, D.E. FREEMAN, AND W.H. PARKINSON

The atmospherically important molecule ozone occurs in the troposphere and stratosphere where the temperature ranges approximately from 200K to 300K. Accurate calculations of the atmospheric transmission in the visible and near ultraviolet regions therefore require laboratory values of the absorption cross section of ozone and its temperature dependence. The major difficulty in performing the cross section measurements of ozone is that the ozone column density is generally not obtainable directly from measurements of the total pressure, because ozone is difficult to prepare free from oxygen and other impurities. We have taken special precautions to prepare pure ozone and prevent its subsequent decomposition. We shall present the absolute cross sections of ozone at several several discrete wavelengths, including the important mercury-line reference wavelength of 253.7 nm, and at the temperatures 295K, 228K and 195K.

This work is supported by grants from NASA and AFGL to the Smithsonian Astrophysical Observatory.

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TG11.

(4:28)

UPPER STATE OF THE SCHUMANN-RUNGE BANDS OF OXYGEN: TRIPLET FINE STRUCTURES FOR $^{16}\text{O}^{16}\text{O}$ AND $^{18}\text{O}_2$

A.S.-C. CHEUNG, K. YOSHINO, D.E. FREEMAN, AND W.H. PARKINSON

Absorption spectra of the Schumann-Runge bands of $^{16}\text{O}^{16}\text{O}$ and $^{18}\text{O}_2$ have been photographed with high resolution in the wavelength region 175-198 nm. For the vibrational levels of $^{16}\text{O}^{16}\text{O}$ with $v' = 9$ and of $^{18}\text{O}_2$ with $v' = 8, 9$ and 11 , the bands become relatively sharp and the triplet structures are partially or completely resolved. Rotational analyses have been reported at Ohio in 1986, and line center positions have now been used in least squares fits to obtain all relevant molecular constants. The spin-spin and spin-rotation constants of the different isotopes will be presented and discussed.

This work is supported by NASA grant NAG 5-484 to Smithsonian Astrophysical Observatory.

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TG12.

(4:40)

PREDISSOCIATION LINE WIDTHS OF THE SCHUMANN-RUNGE BANDS OF $^{16}\text{O}_2$

A.S.-C. CHEUNG, K. YOSHINO, D.E. FREEMAN, J.R. ESMOND, AND W.H. PARKINSON

Non-linear least squares spectral curve fitting has been used to determine predissociation line widths of the Schumann-Runge bands of $^{16}\text{O}_2$. Previously obtained results for the absorption cross sections¹ and molecular constants² were used as data in the fitting procedure. Because the predissociation widths are large compared with the room temperature Doppler widths, Lorentzian profiles were used instead of Voigt profiles. Predissociation widths determined for various vibrational levels will be discussed.

This work is supported by NASA grant NAG 5-484 to Smithsonian Astrophysical Observatory.

¹K. Yoshino, D.E. Freeman, J.R. Esmond and W.H. Parkinson, Planet Space Sci. **31**, 339 (1983).

²A.S.-C. Cheung, K. Yoshino, W.H. Parkinson, and D.E. Freeman, J. Mol. Spectrosc. **119**, 1 (1986).

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TG13.

(4:52)

A HIGH RESOLUTION STUDY OF THE VACUUM ULTRAVIOLET ABSORPTION SPECTRUM OF CS

G. STARK, K. YOSHINO, AND P. L. SMITH

A high-resolution, vacuum ultraviolet absorption study of CS was performed. The CS molecule was produced in a side arm attached to a 25-cm absorption cell, in a silent, a. c. discharge through argon and CS₂. A condensed, a. c. discharge in 400 Torr of krypton was used to produce a background continuum extending from 1250 Å to 1600 Å. Spectra were photographed on a 6.65-m vacuum spectrograph in the first order of a 2400 grooves/mm grating. Four bands (0-0, 1-0, 2-0, 1-1) of the $^{12}\text{C}^{32}\text{S}$ B¹Σ⁺ - X¹Σ⁺ system were observed, plus the 1-0 band heads of $^{13}\text{C}^{32}\text{S}$ and $^{12}\text{C}^{34}\text{S}$. A rotational analysis of the $^{12}\text{C}^{32}\text{S}$ 1-0 band, the only band with resolved rotational structure, was completed. The other bands in the B-X system were observed to be diffuse, presumably because of predissociation of the B¹Σ⁺ state. The derived equilibrium molecular constants of the B¹Σ⁺ state were found to be close in value to those of the ²Σ⁺ ground state of the CS⁺ ion, indicating that the B¹Σ⁺ state is a Rydberg state of CS. All absorption features shortward of the B-X system were found to be diffuse. Descriptions and wavenumbers of these features, which are tentatively identified as CS transitions, are presented.

This work is supported by NASA grant NSG-7304.

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TH1.

(1:30)

VIBRATIONAL ANALYSIS OF PENTAHALIDE METAL COMPLEXES

E. M. NOUR

The vibrational spectra of various pentahalide metal complexes including NbCl_5 , NbBr_5 , MoF_5 and MoCl_5 have been interpreted in details through normal coordinate analysis based on D_{3h} symmetry. The obtained values of force constants for each compound indicate the weakening of the axial M-X' compared with the equatorial M-X bonds. These values are discussed in view of the bonding and structures of these compounds.

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TH2.

(1:47)

INFRARED AND RAMAN SPECTRA OF GASEOUS, LIQUID, AND SOLID METHYL AND METHYL- d_3 VINYL SULFIDE AND THE CONFORMATIONAL STABILITY IN THE GAS PHASET. J. DICKSON AND J. R. DURIG

The Raman spectra (3500-40 cm^{-1}) of gaseous, liquid, and solid methyl and methyl- d_3 vinyl sulfide, $\text{CH}_2\text{CHSCD}_3$, have been recorded, and assignments are provided for the observed bands. From a temperature study of the Raman spectrum of the "light" compound, the enthalpy difference between the low energy *s-cis* conformer and the high energy *gauche* conformer was found to be $750 \pm 68 \text{ cm}^{-1}$ ($2.14 \pm 0.19 \text{ kcal/mol}$). The far infrared spectra of both $\text{CH}_2\text{CHSCH}_3$ and $\text{CH}_2\text{CHSCD}_3$ have been collected at a resolution of 0.1 cm^{-1} for the gases and 1.0 cm^{-1} for the solids. The potential function governing the asymmetric torsion in the gas phase has been determined and the *s-cis/gauche*, *gauche/gauche*, and *gauche/s-cis* barriers are 1803 (5.15 kcal/mol), 508 (1.45 kcal/mol), and 1022 cm^{-1} (2.92 kcal/mol), respectively. The dihedral angle for the *gauche* conformer was determined to be 132° . The barriers to internal rotation of the methyl group have been determined for both conformers in both the gas and solid states.

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TH3.

(2:04)

COMPUTATION OF VIBRATIONAL SPECTRA OF N-ALKANES

B. GALABOV, T. DUDEV, AND J. R. DURIG

Simultaneous calculations of both frequencies and intensities in vibrational spectra, outside of purely theoretical (quantum mechanical) approaches, have been hampered by difficulties in determining transferable intensity parameters from available experimental data. Objectively, intensity parameters are expected to be less transferable compared to force constants because of the higher sensitivity of band intensities to structural changes. There are, however, a number of series of molecules where intramolecular forces and charge distribution are fairly constant, and therefore transferability of both frequency and intensity parameters is expected. A good example in this respect is the normal paraffins. In this paper we present results on the computation of the infrared spectral curves in C_4 , C_5 and C_6 n-alkanes, based on transferable force constants proposed by Shimanouchi et al.¹, and local C-H and C-C intensity parameters determined from experimental gas phase infrared intensities of ethane and propane.² The presence of different conformational forms is also considered.

¹T. Shimanouchi, H. Matsuura, Y. Ogawa and I. Harada, J. Phys. Chem. Ref. Data, 7, 1323 (1978).

²S. Kondo and S. Saeki, Spectrochim. Acta, 20A, 735 (1973).

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TH4.

(2:21)

INFRARED AND RAMAN SPECTRA, CONFORMATIONAL STABILITY, AND VIBRATIONAL ASSIGNMENT OF CYCLOBUTYLGERMANE

T. J. GEYER, T. S. LITTLE, M. DAKKOURI, AND J. R. DURIG

The infrared (3500 to 50 cm^{-1}) and Raman (3500 to 20 cm^{-1}) spectra of gaseous and solid cyclobutylgermane, $c-C_4H_7GeH_3$, have been recorded. Additionally, the Raman spectrum of the liquid has been recorded and qualitative depolarization values have been obtained. From a comparison of the spectra of the fluid phases with that of the solid, it is clear that two stable conformers exist in the fluid phases at ambient temperature. It has been determined that the equatorial conformer is the predominant form at ambient temperature in the gas phase and, from a temperature study of the Raman spectrum in this phase, the enthalpy difference between the equatorial and axial conformers has been determined. Similar studies of the Raman spectrum of the liquid phase have also been carried out, again with the equatorial conformer being thermodynamically preferred and the only conformer present in the solid state. A series of Q-branches have been observed in the low frequency Raman spectrum of the gas and have been assigned to transitions arising from the ring-puckering mode of both conformers. These data have been used to calculate the potential function governing the ring inversion in this molecule.

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TH5.

(2:38)

RAMAN AND FAR INFRARED SPECTRA, CONFORMATIONAL STABILITIES, AND BARRIERS TO INTERNAL ROTATION OF SEVERAL PERFLUOROMETHYL ALCOHOLS

R. A. LARSEN, F. O. COX, B. J. VAN DER VEKEN, AND J. R. DURIG

The Raman (4000 to 50 cm^{-1}) and far infrared (370 to 50 cm^{-1}) spectra of gaseous 1,1,1,3,3,3-hexafluoro-2-propanol ($(\text{CF}_3)_2\text{CHOH}$), 1,1,1-trifluoro-2-ethanol ($\text{CF}_3\text{CH}_2\text{OH}$), as well as the O-D compounds, have been recorded. Particular attention has been given to the O-H stretch and low frequency spectral regions, where evidence is found for the existence of both the *trans* and *gauche* conformers for all of these molecules. From simulations of observed gas phase infrared band profiles, it was possible to assign the OH stretching modes to the *gauche* and *trans* conformers. From relative intensities of the corresponding Raman lines as a function of temperature, the enthalpy difference in the gas phase has been determined for each molecule. Fundamental O-H torsions have been observed for all of the conformers for all of these alcohols. From these observed data, the asymmetric potential function for the internal rotation has been determined for each molecule. Additionally, the respective CF_3 or CH_3 torsional modes have been observed from which internal rotational barriers have been calculated.

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TH6.

(2:55)

INFRARED AND RAMAN SPECTRA, VIBRATIONAL ASSIGNMENT, NORMAL COORDINATE ANALYSIS, AND BARRIER TO INTERNAL ROTATION OF N-CHLORO-N-METHYL METHANAMINE

N. E. LINDSAY, T. J. HIZER, AND J. R. DURIG

The infrared (3200 to 80 cm^{-1}) and Raman (3200 to 10 cm^{-1}) spectra have been recorded for gaseous and solid N-chloro-N-methyl methanamine (dimethyl chloroamine), $(\text{CH}_3)_2\text{NCl}$, and the corresponding deuterium molecules, $\text{CH}_3(\text{CD}_3)\text{NCl}$ and $(\text{CD}_3)_2\text{NCl}$. Additionally, the Raman spectra of the liquids have been recorded and qualitative depolarization values have been obtained. A complete vibrational assignment is proposed, based on the infrared band contours, Raman depolarization values, group frequencies and isotopic shifts. The assignment is supported by a normal coordinate analysis which was carried out by utilizing a modified valence force field to calculate the frequencies and the potential energy distribution. The A' and A'' methyl torsional fundamentals of the $-d_0$ molecule were observed in the infrared spectrum of the gas at 281 and 261 cm^{-1} , respectively, from which the threefold barrier to internal rotation is calculated to be 1658 cm^{-1} (4.74 kcal/mol).

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TH7.

(3:25)

ON THE VIBRATIONAL SPECTRUM OF METHYL NITRITE

HOWARD D. STIDHAM, G. A. GUIRGIS, AND J. R. DURIG

The Raman spectrum of methyl nitrite and methyl-d₃-nitrite is reported in the gas, liquid, and crystalline solid phase. A temperature study of the Raman spectrum of the liquid allowed a direct assignment of the *cis* and *trans* fundamentals. The energy difference between the *cis* and *trans* conformers was estimated from the temperature dependence of two strong Raman bands near 600 cm⁻¹ and agrees well with the NMR value estimated for the liquid (787 cal/mol at 200K by Raman, 803-866 cal/mol by NMR¹).

The room temperature far infrared spectrum of gaseous methyl nitrite and methyl-d₃-nitrite is reported, together with the far infrared spectrum of the polycrystalline materials.

Ab initio geometry optimizations of methyl nitrite at the 3-21G and 6-31G* levels of theory are reported as a function of the N=O torsional angle. Frequency calculations using the 3-21G and 6-31G* levels of theory are reported for the *cis* and *trans* conformers and for a variety of N=O torsional angles near the *cis* and *trans* limits. Considerable molecular relaxation appears in the calculation of optimized geometries, and the possibility of achieving experimental realization of these computational features is discussed.

¹J. P. Chauvel, Jr. and N. S. True, J. Phys. Chem., 87, 1622 (1983).

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TH8.

(3:37)

VIBRATIONAL SPECTRA AND CONFORMATIONS OF (CHLOROMETHYL)THIIRANE

E. J. WURREY, Y.-Y. CHIEN, F. G. ROJAS, P. M. GREEN AND V. F. KALASINSKY

The infrared spectra of (chloromethyl)thiirane in all three phases have been recorded, along with the Raman spectra of this compound in the condensed phases. Since both the liquid phase infrared and Raman spectra exhibit several "doublets" in which one member disappears upon crystallization, it has been concluded that (chloromethyl)thiirane exists in the liquid phase as an equilibrium mixture of two conformers, namely the *gauche*-1 and *gauche*-2 rotameric forms. From the temperature behavior of the Raman intensities of three liquid phase doublets, measured over the range 233 K - 293 K, an enthalpy difference between these two conformers has been determined to be 1.1 ± 0.2 kcal/mole. In addition, a vibrational assignment of the fundamental modes of this molecule has been proposed, and it is in excellent agreement with assignments proposed for similar compounds.

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TH9.

(3:54)

INFRARED SPECTRA OF THE HALOGEN ISOCYANATE AND THIOCYANATE
VAPOR MOLECULES. T. C. DEVORE

Fourier Transform Infrared Spectroscopy has been used to investigate the IR spectra of the X NCO (X = Cl, Br, I, and CN) and the X SCN (X = Cl, Br, I, and SCN) vapor molecules from 4800 cm^{-1} to 400 cm^{-1} . Vibrational frequencies and relative integrated intensities have been determined for each normal mode of vibration which occurs in this region. The similarities and differences observed for each related series of molecules will be discussed.

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TH10.

(4:11)

VIBRATIONAL SPECTRA OF TRANS-1,2-DIFLUOROETHYLENE OXIDE
N. C. CRAIG, C. W. GILLIES, AND K. S. PRANATA

Infrared and Raman spectra of *trans*-1,2-difluoroethylene oxide have yielded a complete assignment of the vibrational fundamentals of this molecule. The frequencies (in cm^{-1}) are: (a) 3086, 1480, 1271, 1162, 1057, 954, 511, 321; (b) 3068, 1320, 1135, 1099, 830, 578, 318. These new results for the O-16 species have led to some adjustments in the previously reported assignments for the O-18 species.¹

Since the O-16/O-18 isotope shift in ν_2 is only 3 cm^{-1} , this mode must be largely CC (and CF) stretching. Symmetric COC stretching is distributed between ν_4 , which shifts 16 cm^{-1} , and ν_6 , which shifts 18 cm^{-1} . Antisymmetric COC stretching must be largely confined to the surprisingly low frequency of 578 cm^{-1} for ν_{14} , which shifts 20 cm^{-1} . These results are a first good example of the effect of heavy atom substitution on the vibrations of a three-membered ring system.

¹J. W. Agopovich, N. C. Craig, C. W. Gillies, and D. J. McGarvey, Paper FA7, 40th Symposium on Molecular Spectroscopy, Columbus, OH (1985).

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Address of Craig and Pranata: Department of Chemistry, Oberlin College, Oberlin, OH 44074

TH11.

(4:23)

MINDO CALCULATIONS AND VIBRATIONAL DYNAMICS OF DL- β -BUTYROLACTONEP. VANEERDEN AND D. MCDERMOTT

This preliminary work discusses the vibrational dynamics and intramolecular force field of DL- β -butyrolactone, a four-membered ring compound sometimes used as a precursor in drug syntheses.

We have initiated a study and determination of possible simple valence force fields (VFF) for DL- β -butyrolactone. One approach is via MINDO calculations. Another approach is with vibrational spectroscopy (i.r. and Raman) and classical normal coordinate calculations.

Except for C-H stretching frequencies and C-H valence stretching constants, the MINDO calculated frequencies are surprisingly close to observed vibrational frequencies. This is unusual for MINDO calculations on a strained ring.

Results of the MINDO and normal coordinate work¹ will be presented and contrasted with a previous study on γ -butyrolactone, which is a five-membered ring.

¹ D. McDermott, J. Phys. Chem. 90, 2569 (1986).

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TH12.

(4:40)

VIBRATIONAL SPECTRA, CONFORMATIONS, AND BARRIERS TO INTERNAL ROTATION IN CYCLOHEXYLSILANE AND PROPYLSILANE

R. C. KENTON, S. SUBRAMANIAM, AND V. F. KALASINSKY

The infrared and Raman spectra of cyclohexylsilane have been recorded for the fluid and solid phases. Spectral intensity changes as a function of temperature for certain of the skeletal ring vibrations indicate the existence of two conformations. These have been tentatively identified as chair conformers with the silyl substituent in the equatorial and axial positions. Sum and difference bands associated with the SiH₂ stretching modes and the SiH₃ torsion have been observed and give a value of 125 cm⁻¹ for the torsion. An additional set of combination bands apparently arise from a low frequency ring vibration. The analysis of this system is underway.

The infrared and Raman spectra of propylsilane have also been investigated in the gas phase. Combination bands associated with the SiH₃ torsion give a torsional frequency of 138 cm⁻¹, and the barrier is calculated to be 1.9 kcal/mole. Another series of combination bands appear to arise from the asymmetric skeletal torsion. Analyses of these bands and the high resolution infrared spectra are underway.

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CALCULATION OF VIBRATIONAL FREQUENCIES FOR LARGE POLYATOMIC MOLECULES USING
THE AM1 HAMILTONIAN

William B. Collier

Recent successes¹ in calculating the vibrational frequencies for polyatomic molecules have encouraged us to try extending this calculational method to the latest semi-empirical hamiltonians. Using the scaled quantum mechanical force field method developed by Pulay et al.², the force fields calculated by the Austin Method 1 (AM1) hamiltonian were scaled. The vibrational frequencies obtained from these scaled force fields yielded good agreement with the observed frequencies. The results for benzene, 9,10-dihydroanthracene, and other selected molecules will be presented.

¹ Harrel Sellers, Peter Pulay, and James E. Boggs, *J. Am. Chem. Soc.*, **107**, 6487 (1985).

² Gabor Pongor, Peter Pulay, Geza Fogarasi, and James E. Boggs, *J. Am. Chem. Soc.*, **106**, 2765 (1984).

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WE1.

(1:30)

**ROTATIONAL SPECTRA OF s-trans AND s-cis GLYOXAL-d, (CHO-CDO)
OBSERVED BY MICROWAVE FOURIER TRANSFORM SPECTROSCOPY**

M. RODLER, M. OLDANI, AND A. BAUDER

Rotational spectra of both conformers of glyoxal-d, have been investigated in the 7.8 - 18 GHz region with a pulsed Fourier transform waveguide spectrometer. The asymmetric isotopic labeling induces a small permanent electric dipole moment in the s-trans conformer. Rotational constants and centrifugal distortion constants have been determined from the frequencies of 20 very weak transitions which have been assigned to s-trans glyoxal-d. Estimates for the deuterium quadrupole coupling constants have been obtained from the hyperfine splittings of two low J transitions.

Rotational constants of the less abundant s-cis glyoxal-d, have been improved and all quartic centrifugal distortion constants have been determined from 16 newly assigned rotational transitions.

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WE2.

(1:47)

**MILLIMETER WAVE SPECTRA OF METHYL- AND DEUTERATED- CYANOACETYLENE, $\text{CH}_3\text{C}_3\text{N}$ AND DC_3N ,
IN SOME EXCITED VIBRATIONAL STATES**

K.M.T. Yamada, G.M. Plummer, M. Bester, G. Winnewisser, M. Tanimoto, and K. Möller

The rotational spectrum of $\text{CH}_3\text{C}_3\text{N}$ in its ν_{12} state has been measured and analyzed for values of J up to 53, allowing the determination of the Coriolis coupling, l-type doubling, and sextic centrifugal distortion constants. Previous work^{1,2} on the related species DC_3N has been extended to 300 GHz and J=35 for several excited bending modes, and a new analysis of these states will be presented.

¹R.A. Creswell, G. Winnewisser, and M.C.C. Gerry, J. Mol. Spec. 65, 420 (1977).

²P.D. Mallinson and R.L. De Zafra, Mol. Phys. 36, 827 (1978).

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WE3.

THE WATER DIMER: THEORY AND MEASUREMENTS

L. H. COUDERT, J. T. HOUGEN, F. J. LOVAS and R. D. SUENRAM

We consider water dimer energy levels using a moderately high-barrier tunneling assumption. This permits us to divide the problem into two parts: one relating to determination of feasible tunneling paths and corresponding tunneling frequencies, the other to determination of how rotational motions modify the tunneling splittings as a function of J and K.

For the first part, based on numerical diagonalizations of one-dimensional multiple-minima vibrational problems, using potential surfaces given by Coker and Watts¹, we find that for the most symmetric isotopic species (H₂O)₂ and (D₂O)₂, two large amplitude motions seem especially feasible. One of these is the (HF)₂-like motion extensively studied in the pioneering work of Dyke *et al.*², with tunneling splittings of approximately 19527 and 1172 MHz, respectively. The other apparently quite feasible motion consists of a 180° internal rotation of the H-donating monomer about the O··H-O bond, accompanied by a simultaneous inversion of the H-accepting monomer's -OH₂ group. Our calculations estimate this splitting for the fully protonated dimer to be of the order of 70000 MHz.

The method³ we use to calculate the J and K dependence of the splittings involves $D_{JK}^J(\chi_p, \theta_p, \phi_p)$ factors which appear in the tunneling matrix elements between two frameworks, and which reflect the mismatch of the rotational wavefunctions. The three angles χ_p, θ_p, ϕ_p were computed for 6 tunneling paths, using a computer program to solve the required coupled ordinary differential equations.

In an attempt to gain further information about tunneling paths not extensively discussed by Dyke *et al.*, we have made new measurements on 1←0 and 2←1 transitions with K=0 for several partially deuterated species of the water dimer. Small splittings, ranging from 4 to 75 MHz were observed. (Because of the nature of the tunneling motions involved, these new data yield only differences in tunneling splittings between the upper and lower state arising from the difference in B values.) Work is in progress and we hope to find the K=1 transitions.

¹D. F. Coker and R. O. Watts, *J. Phys. Chem.* in press.

²Dyke *et al.*, *J. Chem. Phys.* 66, 492-497 and 498-510 (1977), 72 5062-5070 (1980), NATO Conference in Maratea, Italy (1986).

³J. T. Hougen, *J. Mol. Spectrosc.* 114, 395-426(1985).

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WE4.

(2:21)

GLOBAL FIT OF ROTATIONAL ENERGY LEVELS OF THE GROUND VIBRATIONAL STATE OF METHYLAMINE OBTAINED FROM MICROWAVE, FAR-INFRARED PURE ROTATIONAL, AND FAR-INFRARED TORSIONAL BAND TRANSITIONS

N. OHASHI, K. TAKAGI, W. J. LAFFERTY, W. B. OLSON and J. T. HOUGEN

Last year we reported on progress during the preliminary stages of an analysis of the far infrared spectrum of methylamine, using a newly developed effective Hamiltonian (derived essentially from group theoretical considerations) to take into account a variety of effects of the tunneling splittings arising from the methyl group internal rotation and the amino group umbrella motion. Work on the vibrational ground state has now been completed, and we have obtained a fit of about 950 energy level differences with $0 \leq K \leq 19$ and $K \leq J \leq 30$, using 30 molecular parameters. The standard deviation of the fit is 0.00061 cm^{-1} , which is only slightly larger than the expected measurement precision.

Perhaps the most interesting result to emerge from the ground state fit concerns the determination of the structural parameter ρ , which relates the "moment of inertia" of the top to the "moment of inertia" of the whole molecule. One of us found, in earlier fits of microwave data alone¹, that two values of ρ , differing by about 2% were obtained, depending on whether internal-rotation splittings or umbrella-motion splittings were treated. On the basis of the present work, it is now clear that there are two Coriolis terms involving interaction of the large-amplitude angular momentum with the overall angular momentum, since there are two large-amplitude motions in methylamine. In the traditional IAM procedure the value of ρ is determined by requiring the coefficient of the Coriolis term to vanish in the effective Hamiltonian. In the present case we can make the internal-rotation coefficient, or the umbrella-motion coefficient, or some linear combination of the two vanish, but we cannot make both vanish simultaneously. Thus, there is an inherent ambiguity in the value determined for ρ . These and other matters concerning the methylamine spectrum will be discussed.

¹K. Takagi and T. Kojima, J. Phys. Soc. Japan, 30, 1145-1157 (1971).

Address of Ohashi: Department of Physics, Faculty of Science, Kanazawa University, Kanazawa 920, Japan.

Address of Takagi: Department of Physics, Faculty of Science, Toyama University, Toyama 930, Japan.

Address of Lafferty, Olson and Hougen: Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, MD 20899.

WE5.

(2:38)

CALCULATION OF THE TORSIONAL-ROTATIONAL ENERGY LEVELS OF CH_2DXH AND CHD_2XH

Mujian Liu and C. Richard Quade

The torsional-rotational energy levels of CH_2DXH and CHD_2XH have been calculated, where X is either O or S atoms, using an internal axis approach (IAM) for the asymmetric-asymmetric molecules. The internal axis transformation removes the large Coriolis interaction from H_{TR} and places it in the effective H_{T} . However, this transformation introduces additional terms into H_{TR} that depend explicitly upon α .

Solution for the energy levels is considered at three stages. First, the solution of the transformed or effective H_{T} in a free rotor basis. Second, inclusion of the rotational terms from H_{R} (α -independent). And third, inclusion of the terms from H_{TR} , including the α -dependent terms quadratic in the P_i and the small α -dependent terms from the residual Coriolis interaction.

Results from the theoretical formulation and from numerical calculations for the above molecules will be presented.

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WE6.

(2:55)

ROTATIONAL SPECTROSCOPY OF THE EXCITED VIBRATIONAL STATES OF HNO₃R. L. CROWNOVER, R. A. BOOKER, P. HELMINGER, AND F. C. DE LUCIA

This talk will report our work on the millimeter and submillimeter rotational structure of the ν_9 , ν_8 , ν_7 , and ν_6 vibrational states as well as extensions to our earlier work on the ground state. A large amount of data has been obtained and has been fit to Watson's reduced centrifugal distortion Hamiltonian. For each state the rms deviation of the fits was approximately that of the accuracy of the experimental data. For the ν_9 spectrum, structure due to the torsional splitting was resolved. The details of this will be discussed in another talk in this symposium.

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Address of Helming: Department of Physics, University of South Alabama, Mobile, AL 36688

WE7.

(3:25)

MILLIMETER AND SUBMILLIMETER SPECTROSCOPY OF SMALL INTERNAL ROTORS

T. ANDERSON, R. L. CROWNOVER, S. L. SHOSTAK, E. HERBST, AND F. C. DE LUCIA

Small internal rotor molecules play important roles in the millimeter-wave spectra of both interstellar sources and our atmosphere. Indeed, the rotational-torsional spectra of such species are important indicators of the process of star formation in interstellar clouds. In recent years, the Duke Microwave Laboratory has embarked on a study of the rotational-torsional spectra of a variety of fundamental internal rotor species at frequencies up to 1 THz. In this study, both our standard klystron-based spectrometer and a novel broad-band spectrometer have been utilized. Analysis of the data has necessitated improvements to the classical IAM and PAM techniques used to interpret the spectra of internal rotors.

In this talk, recent work on the methanol isotopes $^{13}\text{CH}_3\text{OH}$ and CH_2OD will be discussed. The work on $^{13}\text{CH}_3\text{OH}$ has resulted in the assignment of a number of previously unidentified interstellar lines. In addition, work in progress on several torsional states of $(\text{CH}_3)_2\text{O}$ and of HNO_3 ($\nu_9 = 1$) will be mentioned.

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WE8.

(3:42)

SUBMILLIMETER LASER STARK SPECTROSCOPY SYSTEM

L. JOHNSTON, R. SRIVASTAVA, S. RAJU, G. SUDHAKARAN, J. SARKER, R. BHATTACHARJEE, AND D. HASEROT

A Stark spectrometer and laser system has been developed which can measure Stark spectra of polar molecules with an absorptivity sensitivity of $\alpha \sim 2 \times 10^{-9} \text{ cm}^{-1}$. The accuracy for determining transition frequencies is about one MHz. The Stark plates are made of silvered glass, 60 cm long, spaced 0.05 cm. Stark fields to 60 KV/cm are used. The Stark field is square-wave modulated at 20 Hz. The detector is a Golay cell with quartz window and polyethylene lens optics.

The laser is a direct discharge type, using HCN or DCN, at $\lambda = 337, 311, 195, 190 \mu\text{m}$. Source gases are cyanogen, $(\text{CN})_2$, and H_2 or D_2 , flowing about 10 std cm^3 per minute each. Plano-concave mirror geometry is used, $R_c = 8 \text{ m}$. Inter-mirror distance is 3.7 meters; tube diameter = 10 cm. Mirrors are ground from OFHC copper. Spectral sensitivity is due primarily to stability of laser plasma, and to management of "brown polymer" deposit.

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Address of Raju: Hughes Aircraft Co., P.O.B. 92919, S/C Building 541, Mail Station B326, Los Angeles, CA 90009

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WE9.

(3:54)

GAS PHASE SPECTROSCOPY IN A COLLISIONALLY COOLED CELL NEAR 4K

D. WILLEY, R. L. CROWNOVER, AND F. C. DE LUCIA

We have recently shown that collisions with cold He molecules can be used to cool, under essentially equilibrium conditions, gas phase molecules to very low temperatures¹. The technique is especially advantageous for spectroscopy in the millimeter and submillimeter spectral region. In this region $h\nu > kT$ for very low temperatures and the number of open collisional channels is greatly reduced, thereby simplifying both theoretical calculations and the interpretation of experimental data. The technique is very general, produces strong signals of narrow linewidth, and is applicable to any stable species that is ordinarily studied in this spectral region. In this talk we will describe a new apparatus that we have recently constructed. This new system allows studies at variable temperatures (from the temperature of pumped liquid He up to ambient temperature) and is improved cryogenically from the earlier version. Results from pressure broadening experiments will be described. In addition, its application to the study of weakly bound species, collisional processes in general, and for the purposes of simplifying complex spectra will be discussed.

¹J. K. Messer and F. C. De Lucia, Phys. Rev. Lett. **53**, 2555 (1984).

Address of Willey, Crowover, and De Lucia: Department of Physics, Duke University, Durham, NC 27706

WE10.

(4:11)

MICROWAVE SPECTROSCOPY OF THE ELECTRONICALLY EXCITED STATES
($a^3\Pi_r$ and $a'^3\Sigma^+$) OF COSATOSHI YAMAMOTO AND SHUJI SAITO

The rotational transitions in the metastable electronic states ($a^3\Pi_r$ and $a'^3\Sigma^+$) of CO are observed by a millimeter-wave spectrometer newly constructed at Nagoya University. The spectrum is measured in the region between 80 and 500 GHz. The vibrational satellites are detected up to $v=6$ for the $a^3\Pi_r$ state and up to $v=2$ for the $a'^3\Sigma^+$ state.

The observed spectrum cannot be analyzed by the conventional formulations for the $^3\Pi$ and $^3\Sigma$ states because of the strong perturbation between the a and a' states. The simultaneous analysis including the interaction terms is carried out for the observed transitions and the existing data of the Λ -type doubling transitions in the $a^3\Pi_r$ state.¹ The detailed molecular constants are obtained for the a and a' states.

1. B.G. Wicke et al. J. Chem. Phys. **56**, 5758 (1972).

Address of Yamamoto and Saito: Department of Astrophysics, Nagoya University, Chikusa-ku, Nagoya 464, Japan.

WE11.

(4:28)

**DETECTION AND EQUILIBRIUM MOLECULAR STRUCTURE OF A SHORT-LIVED MOLECULE, HBO,
BY INFRARED DIODE LASER AND MICROWAVE SPECTROSCOPY**

Y. Kawashima, K. Kawaguchi, Y. Endo, and E. Hirota

The IR spectrum of a transient species HBO was observed in the gas phase using a discharge modulation method. The HBO molecule is formed in an ac discharge plasma of a B_2H_6/O_2 or B_2H_6/NO mixture. The ν_3 band origin and the rotational constants of $H^{11}BO$ were determined to be $\nu_0=1825.5610\text{ cm}^{-1}$, $B_0=1.30839\text{ cm}^{-1}$, and $B_3=1.29973\text{ cm}^{-1}$. The microwave spectrum of HBO was subsequently observed using the reaction of diborane with oxygen induced by dc discharge. The rotational, centrifugal distortion, and nuclear quadrupole coupling constants were determined for the $H^{11}BO$ and $H^{10}BO$ species. The rotational transitions in the excited vibrational states, ν_1 , ν_2 , $2\nu_2$ and ν_3 , were also observed for $H^{11}BO$ and $H^{10}BO$. From the equilibrium rotational constants thus obtained, the molecular structure was calculated as $r_e(H-B) = 1.1681(10)\text{ \AA}$ and $r_e(B-O) = 1.2004(3)\text{ \AA}$ with estimated uncertainties in parentheses. The microwave spectra of $D^{11}BO$, $D^{10}BO$, $H^{11}B^{18}O$, and $H^{10}B^{18}O$ were also observed. The rotational transitions in the ν_1 excited state of DBO were not observed at expected frequencies, suggesting that ν_1 was perturbed by a strong Coriolis interaction $\nu_2+\nu_3$.

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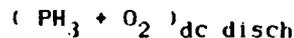
WE12.

(4:45)

The Microwave Spectrum of the PH_2 Radical

Masatoshi Kajita, Yasuki Endo, and Eizi Hirota

The rotational transitions of the PH_2 radical in the ground state were observed in the sub mm-wave region (320~410 GHz). Sixty one fine and hyperfine components were measured for the four Q-branch transitions and one R-branch transition. The PH_2 radical was produced by the following reaction.



From the observed spectra, combined with the data in the mm-wave region (under 300 GHz), infrared region, and optical region obtained by other workers[1], rotational constants, spin-rotation interaction constants, and hyperfine interaction constants were obtained with good accuracy.

Ref. 1) Y.Endo, S.Saito, and E.Hirota. J.Mol.Spectrosc. **97**
204-212 (1983)
and references cited in there

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Myodaiji, Okazaki 444, Japan

WE13.

(4:52)

THE MILLIMETER AND SUBMILLIMETER WAVE SPECTRA OF PROTONATED AND DEUTERATED NITROUS OXIDE

M. Bogey, C. Demuynck, J.L. Destombes and A.R.W. Mc Kellar

A magnetically confined glow discharge has been used to produce protonated and deuterated nitrous oxide in a mixture of N_2O , H_2/D_2 and Ar.

A total number of 63 rotational lines for HON_2^+ and 89 for DON_2^+ characterized respectively by $5 \leq J \leq 18$, $K_a \leq 4$ and $0 \leq J \leq 27$, $K_a \leq 7$ have been observed in the 130 - 405 GHz frequency range. These lines belong to a-type qR - branches and to b-type rR -, qR - and rP - branches. From the analysis of these two types of spectrum, accurate molecular parameters have been derived which are in good agreement with recent IR experiments on HON_2^+ (1). The values obtained for the A rotational constant :

$$A_0 = 625957.716 (52) \text{ MHz for } HON_2^+$$

$$\text{and } A_0 = 349107.385 (14) \text{ MHz for } DON_2^+$$

confirm the recent results of ab initio calculations leading to the conclusion that the preferred site of protonation is at the oxygen atom.

(1) T. Amano, Chem. Phys. Lett., 127, 101 (1986).

Adress of Bogey, Demuynck and Destombes : Université de Lille I, Laboratoire de Spectroscopie Hertzienne associé au CNRS, F - 59655 Villeneuve d'Ascq Cedex, France

Adress of Mc Kellar : Herzberg Institute of Astrophysics, N.R.C., Ottawa K1A 0R6, Canada

WF1.

(1:30)

STUDY OF THE ELECTRONIC GROUND STATE OF NH_2 BY LASER EXCITED FLUORESCENCE FOURIER TRANSFORM SPECTROSCOPY

M. VERVLOET

A large number of spin-rovibronic levels of the upper electronic state of NH_2 have been excited with a single mode rhodamine 6G dye laser. Fluorescence spectra were obtained over a wide spectral range ($12000\text{--}3700\text{ cm}^{-1}$) using a Fourier transform spectrometer. Levels of the bending vibration were observed from $v''=4$ up to 10, showing the reordering of the K-structure at the barrier to linearity; their observed energies are in good agreement with the predictions of Jungen, Hallin and Merer¹, Duxbury and Dixon² and Peric, Peyerimhoff and Buenker³. Numerous vibrational levels involving ν_1 and $2\nu_3$ were also detected and approximate anharmonic parameters have been deduced.

¹C. Jungen, K-E.J. Hallin and A.J.Merer, *Molec.Phys.*, 40, 25 (1980).

²G. Duxbury and R.N. Dixon, *Molec.Phys.*, 43, 255 (1981).

³M. Peric, S.D. Peyerimhoff and R.J. Buenker, *Molec.Phys.* 49, 379 (1983).

Address of Vervloet: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada K1A 0R6.

WF2.

(1:47)

EMISSION BANDS OF THE $\tilde{A}^2A' - \tilde{X}^2A''$ SYSTEM OF HO_2

E. H. FINK, H. KRUSE AND D. A. RAMSAY

Bands of the $\tilde{A}^2A' - \tilde{X}^2A''$ system of HO_2 have been observed in emission from the reaction of metastable O_2 ($^1\Delta_g$) molecules with hydrogen atoms. High resolution spectra have been recorded using a Bomem DA3.002 Fourier transform spectrometer. Rotational analyses have been carried out for the 000-000 and 001-000 bands and improved values for the molecular constants obtained.

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Address of Ramsay: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada K1A 0R6.

WF3.

(2:04)

NEW INFRARED OBSERVATIONS OF THE H₃ MOLECULE

W. A. MAJEWSKI AND J. K. G. WATSON

The new hollow-cathode discharge source described at previous Symposia¹ gives many infrared lines of the H₃ neutral molecule as well as of the vibration-rotation spectrum of the H₃⁺ ion². The former are mostly lines of the known 3s²A₁' → 3p²E' and 3d(2A₁', 2E'', 2E') → 3p²E' electronic transitions^{3,4}, but the higher rotational temperature in the new source makes it possible to extend the previous assignments to higher N levels. The quality of the fit of the spectrum is not significantly improved by introducing additional parameters, suggesting that there are many small but irregular perturbations. A new group of lines near 4300 cm⁻¹ is assigned to the electronic transition 4p²E' → 3s²A₁'. This is the first observation of an n = 4 state of H₃.

¹ Papers TE7 (1985) and RE5 (1986).

² W. A. Majewski, M. D. Marshall, A. R. W. McKellar, J. W. C. Johns, and J. K. G. Watson, J. Mol. Spectrosc., in press.

³ G. Herzberg, H. Lew, J. J. Sloan, and J. K. G. Watson, Can. J. Phys. 59, 428 (1981).

⁴ G. Herzberg, J. T. Hougen, and J. K. G. Watson, Can. J. Phys. 60, 1267 (1982).

Address of Majewski: Department of Chemistry, University of Pittsburgh, Pittsburgh, Pennsylvania 15260.

Address of Watson: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario, Canada K1A 0R6.

WF4.

(2:21)

ROTATIONALLY COLD EMISSION IN THE A²Π₁-X²Π_r SYSTEM OF SO⁺

I. W. MILKMAN, J. C. CHOI, J. L. HARDWICK, and J. T. MOSELEY

The A²Π₁ - X²Π_r band system of SO⁺ has been observed in emission in a corona-excited supersonic expansion of helium and sulfur dioxide. Survey spectra have been recorded at moderate resolution and rotationally analyzed, and selected bands have been recorded and analyzed at high resolution using a 7m focal length grating spectrograph. The analyses provide rotational, vibrational, and spin-orbit constants for several new levels of both electronic states, including bands which involve lower-lying levels of the ground electronic state than had previously been analyzed. In addition, recording spectra as a function of distance from the nozzle allows us to observe the cooling of the rotational structure as the expansion occurs; at about 20 nozzle diameters downstream, the expansion has reached an effective rotational temperature of 20K or less.

Address of Milkman, Choi, Hardwick, and Moseley: Chemical Physics Institute, University of Oregon, Eugene, OR 97403-1274.

WF5.

(2:38)

FORMATION OF O^- IONS IN THE MULTIPHOTON EXCITATION OF NOY. ONO, J. L. HARDWICK, AND J. T. MOSELEY

Formation of the O^- anion in the gas phase has been observed following the multiphoton excitation of nitric oxide at low pressure. By examining both the the multiphoton ionization spectrum and the formation of O^- ions from this molecule as a function of laser frequency, we are able to identify dissociative attachment of photoelectrons to the $A^2\Sigma^+$ electronic state of nitric oxide as the mechanism responsible for formation of negative ions.

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WF6.

(2:55)

INFRARED SPECTROSCOPY OF THE $A^2\Pi_u \leftarrow X^2\Sigma_g^+$ (0,1) HOT BAND OF C_2^- USING TUNABLE DIODE LASER SPECTROMETERDI-JIA LIU, WING-CHEUNG HO, and TAKESHI OKA

Following the high resolution IR spectroscopy of the (0,0) and (1,1) bands in the electronic transition $A^2\Pi_u \leftarrow X^2\Sigma_g^+$ of C_2^- using a difference frequency spectrometer¹, we studied the (0,1) band using a tunable diode laser spectrometer. C_2^- was generated in an *ac* discharge of C_2H_2 and He and was detected using velocity modulation technique. We observed and assigned 25 lines in the 4.7 μm region. These lines were included in the non-linear least squares fit with the (0,0) and (1,1) bands¹. This improved the molecular constants of both electronic states. The following molecular constants have been obtained for the (0,1) band (in cm^{-1}):

T_v	2170.843(24)	B''	1.72153(56)
B'	1.63480(47)	D''	$6.54(94) \times 10^{-6}$
D'	$5.93(72) \times 10^{-6}$	A_D	-0.0001(2)
A	-24.989(19)	p	$-1.2(6) \times 10^{-3}$
q	$-1.13(12) \times 10^{-5}$		
γ	0.004(1)		

Numbers in parentheses are 3σ .

¹ B. D. Rehfuss, D.-J. Liu, B. M. Dinelli, M.-F. Jagod, M. W. Crofton, and T. Oka, 1986 *Symposium on Molecular Spectroscopy*, WG2

Address: Department of Chemistry and Department of Astronomy and Astrophysics, The University of Chicago, Chicago, Illinois 60637

WF7.

(3:12)

FOURIER TRANSFORM SPECTROSCOPY OF THE $A^2\Delta - X^2\Pi$ ELECTRONIC TRANSITION OF THE
JET COOLED CCl FREE RADICAL

L.C. O'BRIEN, C.R. BRAZIER and P.F. BERNATH

The combination of a free radical jet source and a Fourier transform spectrometer promises to be a very powerful tool in unravelling complex emission spectra. We have observed the rotationally cool (30 K) spectrum of the 0-0 vibrational band of the $A^2\Delta-X^2\Pi$ electronic transition of CCl. The spectrum was recorded in emission at high resolution (accuracy of 0.004 cm^{-1} for the strongest lines) using the Fourier transform spectrometer associated with the McMath Solar Telescope. The CCl radical was produced in a corona excited supersonic expansion in a mixture of CCl_4 seeded in helium. The first rotational lines of the six strongest branches (P_1 , Q_1 , R_1 , P_2 , Q_2 , and R_2) were observed. Transitions in three other branches were also detected (R_{12} , Q_{21} and R_{21}), and Λ -doubling was detected in the $^2\Pi_{1/2}$ component of the ground state. The ^{37}Cl isotope structure was only resolved for the R_2 branch. The spectra obtained and the results of the analysis will be discussed.

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WF8.

(3:35)

HIGH RESOLUTION LASER SPECTROSCOPY OF CALCIUM ACETYLIDE (CaCCH)

A.M.R.P. BOPEGEDERA, C.R. BRAZIER and P.F. BERNATH

The calcium acetylide molecule was synthesised in the gas phase by the reaction of calcium vapor with acetylene. Laser-induced fluorescence was used to rotationally analyse the $\tilde{A}^2\Pi-\tilde{X}^2\Sigma^+$ transition of the CaCCH molecule. This molecule proved to be ionic in nature ($\text{Ca}^+\text{-CCH}$) and linear in geometry. The low resolution analysis and the Λ -doubling constant of the CaCCH molecule indicate that the $\tilde{B}^2\Sigma^+$ state is either distant from the $\tilde{A}^2\Pi$ state or dissociative. The molecular parameters of this molecule were determined from the analysis and will be discussed.

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WF9.

HIGH RESOLUTION LASER SPECTROSCOPY OF CaCH_3 AND SrCH_3 C.R. Brazier and P.F. Bernath

We have observed the organometallic free radicals CaCH_3 and SrCH_3 , produced by the gas phase reaction of Ca or Sr metal vapor with $\text{Hg}(\text{CH}_3)_2$ and several other CH_3 containing oxidants. The positions of the $\tilde{\text{A}}^2\text{E}-\tilde{\text{X}}^2\text{A}_1$ and $\tilde{\text{B}}^2\text{A}_1-\tilde{\text{X}}^2\text{A}_1$ transitions have been determined as well as several vibrational frequencies. An upper limit for the bond dissociation energy of 46 kcal/mol (43 kcal/mol) has been determined for CaCH_3 (SrCH_3) from a predissociation in the $\tilde{\text{A}}^2\text{E}$ state. The $\tilde{\text{A}}^2\text{E}-\tilde{\text{X}}^2\text{A}_1$ transition of CaCH_3 has been studied at rotational resolution. Analysis of the spectrum of this prolate symmetric top yields a Ca-C bond length of 2.35 Å.

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WF10.

(4:09)

HIGH RESOLUTION LASER SPECTROSCOPY OF STRONTIUM MONOISOCYANATE, SrNCO L.C. O'BRIEN and P.F. BERNATH

The $\tilde{\text{A}}^2\Pi \leftarrow \tilde{\text{X}}^2\Sigma^+$ transition of strontium monoisocyanate was rotationally analysed at Doppler-limited resolution. Strontium isocyanate was produced by the gas-phase reaction of excited strontium metal vapor ($^3\text{P}_1$ Sr) and hydrogen isocyanate.

The isocyanate ligand was found to be nitrogen bonding to the metal by comparing the SrNCO spectrum with those of the N-bonding strontium monoazide, SrN_3 , and the O-bonding strontium monoethoxide, $\text{SrOCH}_2\text{CH}_3$. SrNCO was found to be a linear, ionic molecule, M^+-NCO , with a low frequency bending vibration ($\sim 40 \text{ cm}^{-1}$) and dense sequence structure. Selective laser excitation with narrow-band fluorescence detection was used to extract the individual branches from the dense rotational and vibrational structure. The spectra obtained and the results of the analysis will be discussed.

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WF11.

(4:21)

HIGH RESOLUTION LASER SPECTROSCOPY OF CaN_3 AND SrN_3 C.R. Brazier and P.F. Bernath

As part of a continuing study of pseudohalide derivatives of Ca and Sr, we have generated the CaN_3 and SrN_3 free radicals by the gas phase reaction of the metal vapor with hydrogen azide. These are linear molecules with an ionic bond between Ca^+ and N_3^- . The $\tilde{\text{A}}^2\Pi-\tilde{\text{X}}^2\Sigma^+$ and $\tilde{\text{B}}^2\Sigma^+-\tilde{\text{X}}^2\Sigma^+$ transitions have been observed and 4 of the 5 vibrational frequencies determined. The presence of an extremely low frequency Sr-N₃ bending mode ($\sim 40\text{cm}^{-1}$) gives rise to extensive sequence structure. A high resolution analysis of the $\tilde{\text{A}}^2\Pi-\tilde{\text{X}}^2\Sigma^+$ transition of SrN_3 has been carried out. The spectrum is extremely dense due to the small rotational constant $B=0.045\text{cm}^{-1}$. The assumption of calculated values for the N-N bond lengths yields a Sr-N distance of 2.25 Å.

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WF12.

(4:38)

OBSERVATION OF THE SCHÜLER BAND OF NH_4 IN A NEUTRALIZED ION BEAM EXPERIMENTW. KETTERLE, P. GRASSHOFF, H. FIGGER, AND H. WALTHER

The Rydberg molecule NH_4 was produced by neutralization of a mass-selected NH_4^+ ion beam. The observation of the main Schüler band near 6635 Å in NH_4 and 6750 Å in ND_4 confirmed the assignment of this band system to NH_4 and ND_4 .

For ND_4 the lifetime of the upper state of the Schüler band, $3p^2F_2$, was determined from the decay of the radiation downstream after the neutralization region. The result of 4.2 ± 1 ns is much shorter than the radiative lifetimes (21 - 28 ns), obtained by various ab initio calculations. This difference as well as the fact that the lifetime of the corresponding state of NH_4 was too short to be measured with our method show that the $3p^2F_2$ state predissociates strongly.

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SPECTROSCOPY OF HELIUM HYDRIDE

W. KETTERLE, A. DODHY, AND H. WALTHER

Discrete spectra of HeH were observed after neutralization of a fast HeH^+ ion beam. A careful determination of Doppler shifts and Doppler broadenings allowed to determine line positions and line broadenings with an accuracy of 0.1 Å.

Accurate molecular constants for the band near 8000 Å were obtained for four isotopic mixtures and are compared with recent ab initio calculations. Isotope effects are discussed.

The linewidth of the band near 8000 Å shows that the $A^2\Sigma^+$ state of HeH predissociates with a lifetime of about 4 ps. The observed intensities of the lines can only be explained if an rotational excitation of HeH^+ of several thousand K is assumed. A first analysis of further bands of HeH in the visible region indicates, that the electronic structure of HeH is very similar to that of the Li atom.

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WG1.

(1:30)

HIGH RESOLUTION FOURIER TRANSFORM SPECTROSCOPY OF ACETYLENE: THE BENDING REGION^{*}

J. J. HILLMAN, G. W. HALSEY, D. E. JENNINGS, AND W. E. BLASS

Acetylene is known to be a constituent in the atmospheres of cool carbon stars based on broad-band and post-dispersed FTS spectra in the 14 micron region. It is also known to be present in many planetary atmospheres. A systematic laboratory study has been undertaken to interpret these astrophysical data on a quantitative basis.

Spectra were recorded with the one-meter FTS located at the McMath solar telescope at the National Solar Observatory. The FTS was used in the double-pass mode to produce an unapodized spectral resolution of 0.0025 cm^{-1} . The spectra were calibrated with respect to NH_3 and are believed to be accurate to at least 0.0001 cm^{-1} . Three optical densities were recorded, all at room-temperature ($294 \pm 1 \text{ K}$): 0.57- , 59.6- , and 1257.6 Torr-cm .

We shall discuss the interpretation of approximately 1500 assigned lines. GSCD analysis has resulted in refinement of the ground state, the fundamental bending modes, and the associated hot bands of $^{12}\text{C}_2\text{H}_2$ and $^{12}\text{C}^{13}\text{CH}_2$.

^{*} This research is supported, in part, by the NASA Planetary Atmospheres Program.

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WG2.

(1:47)

THE ν_3 SPECTRAL REGION OF CS_2 : SPECTRA

V. Malathy Devi, Guy Guelachvili, D. Chris Benner and K. Narahari Rao

Two spectra of a natural isotopic sample of CS_2 have been obtained in the 1440 to 1560 cm^{-1} spectral region with the high information Fourier transform spectrometer at Orsay. These spectra have a resolution of 0.0054 cm^{-1} and a signal to noise ratio of 1000. In addition, over 200 diode laser scans of portions of the most crowded region, 1494 to 1535 cm^{-1} were also obtained. These diode laser scans provide nearly complete frequency coverage in this region and have been obtained with both a natural isotopic sample and a sample enriched with the rarer isotopes. The signal to noise ratio of these scans is generally 1000 to 2000 and the resolution 0.003 cm^{-1} . Positions of isolated strong spectral lines on the FTS spectra can be measured with a precision of 0.00002 cm^{-1} . These positions have been used to calibrate the frequency scales of the diode laser spectra. The diode laser scales are accurate to a precision of 0.0001 cm^{-1} , being limited by how well the laser fringes can be fit.

The two types of spectra compliment each other well. The broad frequency coverage and precise positions of the FTS spectra facilitate identification of the spectral lines and calibration of the frequency scales of the diode laser spectra. The diode laser spectra, on the other hand, resolve blends and, since the position measurements are not limited by the resolution or signal to noise, provide more accurate positions for weaker spectral lines.

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WG3.

(1:59)

THE ν_3 SPECTRAL REGION OF CS_2 : ASSIGNMENTS AND MOLECULAR CONSTANTSD. Chris Benner, V. Malathy Devi, Guy Guelachvili and K. Narahari Rao

Positions of a few thousand CS_2 spectral lines on the Fourier transform and diode laser spectra by Malathy Devi et al.¹ have been measured. Numerous $\Delta v_3 = 1$ transitions involving ^{32}S , ^{33}S , ^{34}S , ^{12}C and ^{13}C have been identified and assignments made for over 20 bands. Molecular constants have been derived for the identified bands and comparisons of these constants with the previously reported values for nine bands will be made. Comparison to theoretically predicted values will be made for all of the bands.

¹V. Malathy Devi, G. Guelachvili, D. C. Benner and K. Narahari Rao, this session.

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WG4.

(2:11)

AIR-BROADENED AND NITROGEN-BROADENED WIDTH COEFFICIENTS AND PRESSURE SHIFTS IN THE ν_4 AND ν_2 BANDS OF $^{12}\text{CH}_4$ C. P. RINSLAND, V. MALATHY DEVI, M. A. H. SMITH, AND D. CHRIS BENNER

Air-broadened and N_2 -broadened width coefficients and pressure shifts of transitions in the ν_4 and ν_2 bands of $^{12}\text{CH}_4$ have been measured from room temperature 0.01 cm^{-1} resolution absorption spectra recorded at a signal-to-rms noise of ~ 500 with the Fourier transform spectrometer in the McMath telescope of the National Solar Observatory. Total pressures of up to 550 Torr were employed with absorption paths of 5 to 150 cm and a CH_4 volume mixing ratio of 2.5% or less. A nonlinear least-squares spectral fitting technique has been utilized to retrieve the positions, intensities, and the halfwidths of several hundred spectral lines from each of the 22 measured spectra. Unshifted line positions were determined from additional FTS spectra of pure CH_4 at low pressure, and all spectra were calibrated using well-determined H_2O standards near $7 \mu\text{m}$. The measured positions and widths from the various spectra have been combined to determine the broadening coefficients ($\text{cm}^{-1} \text{ atm}^{-1}$) and pressure shifts ($\text{cm}^{-1} \text{ atm}^{-1}$) and their uncertainties. Lines up to $J'' = 18$ have been analyzed.

The experimentally determined halfwidths and pressure shifts will be presented and compared with previously published measurements and calculations.

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WG5.

(2:23)

AIR-BROADENED LORENTZ HALFWIDTHS IN THE ν_4 BAND OF $^{13}\text{CH}_4$ USING A FOURIER TRANSFORM SPECTROMETER

V. Malathy Devi, C. P. Rinsland, M. A. H. Smith and D. Chris Benner

Room-temperature air-broadened Lorentz halfwidths for more than 150 transitions (for $J \leq 15$) in the ν_4 fundamental of $^{13}\text{CH}_4$ between 1200 and 1380 cm^{-1} have been determined by analyzing 0.01- cm^{-1} resolution spectra recorded with the Fourier transform spectrometer in the McMath telescope of the National Solar Observatory on Kitt Peak. A 99% ^{13}C -enriched $^{13}\text{CH}_4$ sample diluted to $\approx 0.5\%$ by mixing the sample with approximately 200, 350 and 505 Torr of dry air was used in a 50-cm long absorption cell. The halfwidths were determined using nonlinear least-squares spectral curve fitting. The measured air-broadened halfwidths are compared with values determined previously for several transitions in the same band using a tunable diode laser spectrometer system.¹ Comparisons with identical transitions in the ν_4 band of $^{12}\text{CH}_4$ will also be made.

¹V. Malathy Devi, C. P. Rinsland, M. A. H. Smith and D. C. Benner, Appl. Optics, 24, 3321-3322 (1985).

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WG6.

(2:35)

ABSOLUTE LINE INTENSITIES OF $^{12}\text{CH}_3\text{D}$ AND PRESSURE BROADENING COEFFICIENTS FOR $\text{CH}_3\text{D}-\text{N}_2$ AND $\text{CH}_3\text{D}-\text{H}_2$ MIXTURES

K. P. Carten, S. H. Kensinger, R. W. Lovejoy, and C. Chackerian, Jr.

Absolute intensities of several P-branch, Q-branch, and R-branch lines of the ν_2 infrared band of pure CH_3D have been measured at room temperature using a tunable diode laser spectrometer. These experimental results will be compared to calculated values. Pressure broadening coefficients of CH_3D by N_2 were measured to reproduce conditions in the earth's stratosphere. Similar measurements of CH_3D by H_2 were made to simulate Jupiter's atmosphere.

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WG7.

(3:05)

TORSIONAL EFFECTS IN THE HAMILTONIAN AND DIPOLE MOMENT OF METHYL SILANE LIKE MOLECULES

N. MOAZZEN-AHMADI AND I. OZIER

The effect of internal rotation on the redundancies in the torsion-rotation Hamiltonian H_{TR} and on the dipole moment operator for methyl silane like molecules (G_{18} symmetry) is examined. It is shown that H_{TR} contains a new term with selection rules $\Delta K = \pm 3$, $\Delta \sigma = 0$, and $\Delta v_T = \text{arbitrary}$, where v_T and σ label the torsional levels and sub-levels, respectively. As a result, the distortion dipole moment μ_D which arises from mixing of $\Delta K = \pm 3$ level in molecules with C_{3v} symmetry cannot, in systems like methyl silane, be ascribed entirely to centrifugal distortion but can contain a significant contribution from torsional effects. Furthermore, new transitions can appear in the pure torsional bands which may be strong enough to observe in low barrier molecules. Finally, the physical origin of the leading torsional terms in the dipole moment expression which give rise to pure torsional band is described.

This work was carried out at: Department of Physics, University of British Columbia, 6224 Agriculture Road, Vancouver, B.C., V6T 2A6, Canada.

WG8.

(3:22)

THE TORSIONAL SPECTRUM OF CH_3CH_3 AT HIGH RESOLUTIONN. MOAZZEN-AHMADI, H.P. GUSH, M. HALPERN, H. JAGANNATH, A. LEUNG, AND I. OZIER

The torsional spectrum of ethane has been studied between 225 and 330 cm^{-1} at a resolution of 0.015 cm^{-1} using Fourier transform spectroscopy. Observations were made at room temperature, with an absorption path length of 124 m and a pressure of 107 torr. In lowest order, the transition dipole moment arises from Coriolis mixing of the vibrational fundamentals into the ground vibrational state. The P, Q, and R branches of all four torsional sublevels have been measured for the two bands $v_4 = 1 \leftarrow 0$ and $v_4 = 2 \leftarrow 1$. By analysing over 300 lines in the P and R branches of the fundamental, a good fit was obtained by adapting the torsion-rotation Hamiltonian used for CH_3SiH_3 .¹ Values will be presented for the height V_3 of the six-fold potential barrier, the value of the B rotational constant, and three rotation-torsion distortion constants. Work is underway to extend the analysis to the Q branch of the fundamental and to the three branches of the hot band.

¹ - M. Wong, I. Ozier, and W.L. Meerts, J. Mol. Spectrosc. 89, 111 (1983).

This work was carried out at: Department of Physics, University of British Columbia, 6224 Agriculture Road, Vancouver, B.C., V6T 2A6, Canada.

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WG9.

(3:39)

TORSIONAL SPLITTINGS IN $\nu_9 + \nu_4$ OF C_2H_6

J. Susskind, W. E. Blass, D. C. Reuter, and G. W. Halsey

Torsional splittings in the torsional hot band $\nu_9 + \nu_4 - \nu_4$ of C_2H_6 have been measured in the P and R branch sub-bands from R_{15} to P_{16} . Every transition is split into a non-degenerate and a doubly degenerate component with splittings generally near 0.086 cm^{-1} . Individual splittings vary between extremes of 0.235 cm^{-1} and -0.079 cm^{-1} (splitting is of opposite phase). The detailed behavior of the splitting is described quantitatively by the zeroth order torsional Hamiltonian for ν_9 ,

$$H_{\text{TOR}}^{(9)} = A P_Y^2 + \frac{V_6^{(9)}}{2} (1 - \cos 6Y),$$

together with the xy Coriolis Interaction operator⁽¹⁾

$$H_{\text{COR}} = -2B\zeta_{4,9}^{xy} \left[(2A)^{1/2} P_Y (J_{-Q_{9+}} + J_{+Q_{9-}}) - (2A)^{-1/2} \frac{\sin 6Y}{6} (J_{-P_{9+}} + J_{+P_{9-}}) \right]$$

connecting $\nu_9 + \nu_4$ and the excited torsional states $2\nu_4$, $3\nu_4$, $4\nu_4$, $5\nu_4$, and $6\nu_4$. Of these, interactions with the nearby $4\nu_4$ and $5\nu_4$ states contribute very significantly to the splittings. Interactions of $\nu_9 + \nu_4$ with $n\nu_4$ (n -odd) are nominally forbidden ($g + u$) in the high barrier limit, corresponding to a rigid molecule. Such interactions are not strictly forbidden, however, but are allowed only in doubly degenerate torsional states, with matrix elements which increase rapidly with torsional quantum number. The zeroth order splitting (0.086 cm^{-1}) and the Coriolis interaction constant ($\zeta_{4,9}^{xy}$) and torsional matrix elements consistent with the spectra are predicted extremely well by the coefficients determined from the analysis of splittings in the ν_9 band of ethane⁽¹⁾.

¹ J. Susskind, D. Reuter, D. E. Jennings, S. J. Daunt, W. E. Blass, and G. W. Halsey. J. Chem. Phys., 77, 2728 (1982)

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WG10.

(3:56)

DETERMINATION OF TORSIONAL STATE ROTATIONAL CONSTANTS FROM LOWER STATE COMBINATION DIFFERENCES IN $\nu_9 + \nu_4 - \nu_4$ OF C_2H_6

W. E. BLASS, G. W. HALSEY, JOEL SUSSKIND, D. C. REUTER AND D. E. JENNINGS

Using the assigned transitions in $\nu_9 + \nu_4 - \nu_4$ from the 0.0025cm^{-1} resolution spectra observed using the FTS spectrometer at the National Solar Observatory, in excess of 550 lower state combination differences have been analyzed. Each torsional state has been treated separately yielding values for $B_{\tau, \sigma}$, $D_{\tau, \sigma}$ and D_{JK} (variation in D_{JK} as a function of σ was not determined by the data.)

	B_0	$10^3 D^J$	$10^3 D^{JK}$	Std.Dev.	N/ZW/N
$\sigma = 0$	0.6605099(73)	0.10261(68)	0.274(16)	0.00088	92/ 96
$\sigma = 1$	0.6605005(44)	0.10214(36)	0.272(18)	0.00068	179/182
$\sigma = 2$	0.6604930(54)	0.10158(49)	0.273(12)	0.00088	184/190
$\sigma = 3$	0.6604846(77)	0.10147(74)	0.268(18)	0.00074	83/ 87

All quantities except σ and N/NZW in units of cm^{-1} . N/NZW is the number of non-zero weighted combination differences and the total number of combination differences used in the analysis. Weights used were modified bi-weights.

Even though the moments of inertia of ethane are independent of torsional coordinates one would expect the rotational constants to have an effective torsional dependence as a result of interactions with other vibrations. This dependence may be expressed as a Fourier series in $(1 - \cos(6\gamma))$. We have used a truncated model of the form

$$B_{\tau, \sigma} = B + \delta B \langle \tau, \sigma | \cos(6\gamma) | \tau, \sigma \rangle$$

Using this model and the results given above we have been able to predict $B_{\tau, \sigma}$ for the ground state and the $\tau=3$ state that induces the large splittings seen in ν_9 .

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WG11.

(4:13)

ANALYSIS OF THE 17μ HIGH RESOLUTION SPECTRUM OF ν_9 OF C_2D_6

F. VILLAMAGNA, S. J. DAUNT AND W. E. BLASS

A 0.004cm^{-1} (nominal) resolution spectrum of ν_9 of C_2D_6 has been observed using an FTS spectrometer. The optical density was 180 torr-cm in a 15 cm cell. Over 1000 transitions have been assigned and preliminary ground state constants have been obtained suggesting a relative precision of better than 0.0006cm^{-1} in the observed data. An $l(2,2)$ resonance analysis has been carried out with no indication of significant model problems at the apparent resolution of the data. Final analysis results will be presented for both the ground state parameters and the ν_9 parameters.

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WG12.

(4:25)

PRELIMINARY INTERPRETATION OF THE 15 μ m SPECTRUM OF ν_{12} OF CH₃CD₃

F. VILLAMAGNA, W. E. BLASS, D. C. REUTER AND S. J. DAUNT

A 0.004cm⁻¹ (nominal) resolution spectrum of ν_{12} of CH₃CD₃ has been observed using an FTS spectrometer. The optical density was 330 torr-cm in a 15 cm cell. Over 1000 transitions have been assigned and preliminary ground state constants have been obtained suggesting a relative precision of better than 0.0006 cm⁻¹ in the observed data. Even though the observed spectrum is slightly pressure broadened exhibiting an apparent resolution of approximately 0.008cm⁻¹, torsional doublets have been observed for J values as low as eight. A model based on torsional splittings enhanced by resonances between ν_{12} and several torsional states is being developed. The state of the interpretation and analysis will be presented.

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WG13.

(4:37)

Frequency Stabilization of a Tunable Diode Laser
Using an Internally Coupled Confocal Etalon

R.D. Schaeffer and W. Jalenak, Spectra Physics, Laser
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01730 USA

Recent trends in molecular spectroscopy have pointed out the need for improvement of experimental techniques to reduce frequency jitter of the diode, enhance signal to noise ratio, and provide a better relative reference marker for frequency scaling. All three of these requirements have been met with the introduction by Laser Analytics, Inc. of an internally coupled confocal Fabry Perot resonator which can be line locked to an infrared fringe by servo looping back to the laser current source through a lock in amplifier. Significant signal improvements have been seen in the laboratory, and current work suggests that the future will reveal more interesting benefits of such a technique. Hardware description, basic theory, and experimental data will be presented.

WH1.

(1:30)

VIBRATIONAL OPTICAL ACTIVITY OF CHLOROFLUOROACETIC ACID

M.A. Davies, J. Calienni, U. Gunnia and M. Diem

Raman Optical Activity (ROA) in the 200 - 1200 cm^{-1} region, and infrared Vibrational Circular Dichroism (VCD) in the 1000 - 3000 cm^{-1} region, have been observed for neat chlorofluoroacetic acid and chlorofluoroacetate in aqueous solution. These species are probably the smallest systems studied to date by vibrational optical activity (VOA). Thus, the interpretation of the VOA spectra of these molecules provides new insight on the origin of VOA in terms of the atomic displacements.

The VOA measurements have been accompanied by detailed vibrational measurements on chlorofluoroacetic acid, deuteriochlorofluoroacetic acid, chlorofluoroacetate and deuteriofluoro-chloro acetate. Calculated VCD intensities, based on a Urey-Bradley force field, will be compared to the experimental values.

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WH2.

(1:47)

A DEDICATED FOURIER TRANSFORM INSTRUMENT FOR THE MEASUREMENT OF VIBRATIONAL CIRCULAR DICHROISM

Günter Georg Hoffmann,* Bernhard Schrader, and Günther Snatzke

Vibrational circular dichroism can be measured either with dispersive instruments or with FTIR spectrometers. Using the dispersive approach, commercially available instruments could not be used after appropriate modification. Dedicated instruments had to be built in order to account for the weak signals to be measured. On the contrary, FTIR instruments are much more sensitive than dispersive instruments and considerably more expensive than dispersive instruments, so that until now commercially available instruments were equipped with the appropriate auxiliary devices to allow the measurement of VCD. In this paper we wish to describe a dedicated VCD-interferometer, which is designed to minimize the number of optical elements, thus hopefully reducing artifacts in VCD spectra.

In the dedicated instrument an off-axis parabolic mirror collects the light of a global into a parallel beam, which is fed into a modular Michelson interferometer (design adapted from Horlick, Applied Spectroscopy 32 [1978] 38). In our new design the outgoing parallel beam is directly focussed onto the detector, on its way travelling through the linear polarizer, photoelastic modulator and sample. This design thus avoids the possible alteration of the polarization state of the measured light and thus eliminates some important sources of artifacts.

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This work was supported by the "Minister für Wissenschaft und Forschung des Landes Nordrhein-Westfalen."

WH3.

(2:04)

CH- AND CD-STRETCHING VIBRATIONAL CIRCULAR DICHROISM IN (S,S)-[2,3-²H₂]OXIRANE

L. A. NAFIE, T. B. FREEDMAN, M. G. PATERLINI, J. M. SCHWAB AND T. RAY

Vibrational circular dichroism spectra in the carbon-hydrogen and carbon-deuterium stretching regions of (S,S)-[2,3-²H₂]oxirane have been obtained. This is the simplest molecule for which VCD has been recorded to date. The spectra, which consist of a positively biased (+,-) couplet the CH-stretching region and a negatively biased (+,-) couplet in the CD-stretching region, can be understood in terms of the coupled oscillator and ring current mechanisms of VCD.

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WH4.

(2:16)

VIBRATIONAL CIRCULAR DICHROISM SPECTRA OF (S)-4-BENZYL-2-OXAZOLIDINONE IN CDCl₃ SOLUTION

R. L. WOOD, T. B. FREEDMAN, L. A. NAFIE

Vibrational circular dichroism (VCD) spectra of (S)-4-benzyl-2-oxazolidinone in CDCl₃ in the C-H, N-H, and C=O stretching and C-H and N-H bending regions will be presented. All VCD spectra show a distinct bias. Analysis of these spectra, based on an application of the ring current mechanism, leads to the determination of the conformation of this molecule in solution. Only one ring conformation is consistent with the sign of the VCD signal in all spectral regions.

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WH5.

(2:28)

VIBRATIONAL CIRCULAR DICHROISM IN THE CH-STRETCHING REGION OF (+)-(3R)-METHYLCYCLOHEXANONE AND CHIRAL DEUTERATED ISOTOPOMERS

T. B. FREEDMAN, J. KALLMERTEN, E. D. LIPP AND L. A. NAFIE

An analysis of the CH-stretching FTIR and vibrational circular dichroism (VCD) spectra of (3R)-methylcyclohexanone and its chiral -2,6-d₄, -4-d₂, -5-d₂ and methyl-d₃ isotopomers, and the FTIR spectrum of racemic 3-methylcyclohexanone-3-d₁ will be presented. Band assignments to local CH stretching motions have been made by using Fourier self-deconvolution to clarify the effects of specific deuteration on the FTIR spectra and by analyzing the strong Fermi resonance interactions. Nearly all the VCD features in the five chiral isotopomers can be attributed to the coupling of chirally oriented CH oscillators on adjacent carbon atoms. The analysis can be readily extended to the interpretation of the VCD spectra in molecules containing the chiral CH₂CH₂C*H chromophore previously considered by Laux, et al.¹

¹L. Laux, V. Pultz, S. Abbate, H. A. Havel, J. Overend, A. Moscovitz and D. A. Lightner, J. Am. Chem. Soc. 104, 4276 (1982).

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WH6.

(2:45)

ABSORPTION AND CIRCULAR DICHROISM DUE TO BENDING VIBRATIONS OF A_2B_2 MOLECULES OF C_2 SYMMETRY.**P. L. POLAVARAPU**

The expressions for vibrational absorption and circular dichroism intensities are derived which require only the knowledge of molecular geometry and Sayvetz conditions. Three different cases are considered. (a). When partial charges are assumed to follow the nuclei, and charge flux is negligible, the dissymmetry factor for symmetric bending vibration is about two orders of magnitude larger than that for antisymmetric bending vibration. (b). When fixed partial charge contributions are negligible and charge flux along B-B bond is of the same order as that along A-B bond, the dissymmetry factors for symmetric and antisymmetric bending vibrations are of the same magnitude, for molecules with $\sim 60^\circ$ dihedral angle. (c). When fixed partial charge contributions are negligible and charge flux along A-B bonds is greater than that along B-B bond, the dissymmetry factors for symmetric and antisymmetric bending vibrations follow $\tan^2 \Theta$ relation. The latter two points are also applicable to the two A-B stretching vibrations. Details of the theoretical formulation and of the above summary will be discussed in this presentation.

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WH7.

(3:15)

FOURIER TRANSFORM IR-VIBRATIONAL CIRCULAR DICHROISM AND THE PROBLEM OF ARTIFACT SIGNALS**P. MALON AND T. A. KEIDERLING**

FTIR-VCD has become a popular method of obtaining vibrational circular dichroism (VCD) data since its recent development by Nafie and coworkers. We have just assembled a new FTIR-VCD instrument based on a Digilab FTS-60 with some design improvements that suggest an apparent solution of the baseline problem. In the FTIR-VCD data presented to date, it has always been necessary to have a racemic mixture or opposite enantiomer to correct for baseline artifacts which were correlated to absorption bands and often were much larger than the VCD signal. By correcting the baseline through optical alignment and modification to a lens system from the standard focussing mirror, we have minimized these artifacts to the point where, under favorable conditions, no baseline correction is needed other than solvent. Examples of FTIR-VCD on "standard" molecules will be presented, both with and without the artifacts. Such a development is very important for the application of FTIR-VCD to biological systems such as peptides and proteins where only one enantiomer is available. We have also found this baseline correction to affect the observed FTIR-VCD band-shape, which brings these results into closer agreement with our previously published dispersive VCD results. The latter are less affected by baseline artifacts than were the original FTIR-VCD results. These developments suggest that the deconvolution of FTIR-VCD is at present premature, since the conditions of measurement affect the band-shape, and that determines the resolution enhanced result.

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WH8.

(3:32)

MVCD OF PORPHYRINS AND METALLOPORPHYRINS

P. V. CROATTO AND T. A. KEIDERLING

We have measured the magnetic vibrational circular dichroism (MVCD) of tetraphenylporphine and octaethylporphine and the metal substituted porphyrins (Mg, Mn, Fe, Co, Ni, Cu, Zn, Ru). The spectra are dominated by large positive A terms in the mid-IR corresponding to ring CC and CN stretches. The A_1/D_0 values determined from moment analysis are much larger than seen in benzene and substituted benzenes. This change is consistent with the vibronic coupling model of MVCD previously reported.

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WH9.

(3:44)

THEORIES OF VIBRATIONAL ROTATIONAL STRENGTHS. P.J. STEPHENS

The fundamental equation for the rotational strength of a vibrational transition derived by Stephens [1] can be transformed into several alternative forms. Atomic polar and axial tensors can be related to electric and electromagnetic nuclear shielding tensors defined by Lazzeretti and Zanasi [2], permitting rotational strengths to be expressed in terms of nuclear shielding tensors. Alternative choices of gauge also provide new forms of the equation. A new gauge choice, referred to as the Distributed Origin Gauge, is introduced. In this gauge, Stephens' equation contains two terms, the P.L. and the P.RxP terms. Neglecting the former term yields the P.RxP approximation, which is formally identical to the Atomic Polar Tensor Model equation of Freedman and Nafie [3]. The Fixed Partial Charge (FPC) equation of Schellman [4] and the coupled oscillator (CO) equation of Holzwarth and Chabay [5] are approximations to the P.RxP equation.

1. P.J. Stephens, *J. Chem. Phys.* **89**, 748 (1985).
2. P. Lazzeretti and R. Zanasi, *Phys. Rev. A* **33**, 3727 (1986).
3. T.B. Freedman and L.A. Nafie, *J. Chem. Phys.* **78**, 27 (1983).
4. J.A. Schellman, *J. Chem. Phys.* **58**, 2882 (1973).
5. G. Holzwarth and I. Chabay, *J. Chem. Phys.* **57**, 1632 (1972).

Address of Stephens: Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482.

WH10.

(4:01)

CALCULATIONS OF VIBRATIONAL ROTATIONAL STRENGTHS. P.J. STEPHENS, K.J. JALKANEN, R.W. KAWIECKI, R.D. AMOS, N.C. HANDY, P. LAZZERETTI AND R. ZANASI

Calculations of vibrational rotational strengths using the multiple equations discussed in the previous paper at the SCF level are reported for a range of small, chiral molecules including NHDT, NH_2NH_2 and trans-dideuteriocyclopropane. The basis set and origin dependence of the results and their accuracy relative to the Hartree-Fock limit are discussed. The relative accuracies of different equations for rotational strengths are compared. The degree to which the P.RxP, FPC and CO equations are reliable approximations is examined.

Address of Stephens, Jalkanen and Kawiecki: Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482.

Address of Amos and Handy: Department of Theoretical Chemistry, Cambridge University, Cambridge, United Kingdom.

Address of Lazzeretti and Zanasi: Dipartimento Di Chimica, Universita Degli Studi Di Modena, 41100 Modena, Italy.

WH11.

(4:18)

VIBRATIONAL CIRCULAR DICHROISM OF S-(-)-PROPYLENE OXIDE. P.J. STEPHENS, R.W. KAWIECKI, F. DEVLIN,
R.D. AMOS, N.C. HANDY AND M.A. LOWE

The vibrational circular dichroism (VCD) of S-(-)-propylene oxide (neat liquid and CS₂ and CCl₄ solutions) over the range 3200-650 cm⁻¹ is reported. Dispersive VCD instrumentation incorporating sub-77°K detectors has been utilized for these measurements. The results are compared with calculations of the VCD spectrum using Stephens' equation. SCF calculations of atomic polar and axial tensors are carried out using analytical derivative methods for a wide range of basis sets and molecular geometries. Scaled SCF force fields calculated for a range of basis sets are used to obtain vibrational frequencies and normal coordinates.

Address for Stephens, Kawiecki and Devlin: Department of Chemistry, University of Southern California, Los Angeles, CA 90089-0482.

Address for Amos and Handy: Department of Theoretical Chemistry, Cambridge University, Cambridge, United Kingdom.

Address for Lowe: Department of Chemistry, Boston University, Boston, MA 02215.

WH12.

(4:35)

AN INTERPRETATION OF IR AND VCD INTENSITIES BASED ON NUCLEAR ELECTROMAGNETIC SHIELDINGS

P. LAZZERETTI AND R. ZANASI

The electrons of a molecule perturbed by external radiation induce dynamic electric and magnetic fields at the nuclei, superimposing to those of the perturbation.

This behavior can be interpreted in terms of electromagnetic shieldings of the electrons on the nuclei, which are acted upon by effective Lorentz forces driving the vibrational motion.

The absorption intensity of IR and VCD bands can be related respectively to electric and electro-magnetic nuclear shieldings, which are connected with electric polarizability, magnetizability, optical rotatory power and other second-order properties via equations discussed in the following talk.

Address: Dipartimento di Chimica, Università degli Studi, Via Campi 183, 41100 -Modena, Italy.

RA1.

(8:30)

LASER INDUCED FLUORESCENCE SPECTRUM OF COLD METHOXY RADICAL

STEPHEN C. FOSTER, XIANMING LIU, PRABHAKAR MISRA, LIAN YU, CRISTINO P. DAMO, AND TERRY A. MILLER

The methoxy radical has been the subject of numerous theoretical and experimental spectroscopic studies. This interest arises, in part, because of its importance in combustion systems and in the chemistry of the upper atmosphere. Perhaps more importantly, the spin-orbit splitting and Jahn-Teller distortions of its 2E electronic ground state are predicted to be significant. Thus this radical provides an excellent test of our current understanding of the interaction between these effects.

We have produced rotationally cold ($<2K$) methoxy radicals by 248 nm photolysis of methyl nitrite (CH_3ONO) seeded in a helium free-jet expansion. A laser excitation spectrum of the $\bar{A} \leftarrow \bar{X}$ system was recorded with a frequency-doubled dye laser and showed completely resolved rotational structure. Detailed information about the ground-state vibrational structure has also been obtained by dispersing the fluorescence from laser-excited single rovibrational levels of the $\bar{A}{}^2A_1$ state. The implications of these spectral results for the electronic and geometric structure of the molecule will be discussed.

Address: Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, Columbus, Ohio 43210.

RA2.

(8:47)

LASER INDUCED FLUORESCENCE OF FURAN CATION PRODUCED BY MULTIPHOTON IONIZATION IN A SUPERSONIC JET

R. S. Smith, L. F. DiMauro, and T. S. Sears

The LIF spectrum of the $X \rightarrow B$ transition of jet cooled furan cation is reported. The cation is formed by multiphoton ionization of furan seeded in a jet expansion. Vibrational analysis is presented for both electronic states of the cation and compared with photoelectron spectra. The formation mechanism of the cation in a jet environment is also discussed.

Address of DiMauro and Smith: Department of Physics, Louisiana State University, Baton Rouge, LA 70803.

Address of Sears: Department of Chemistry, Brookhaven National Laboratories, Upton, NY 11973.

RA3.

(9:04)

LIFETIMES OF THE LOWEST EXCITED STATES OF THE CYCLOPENTADIENYL AND THE MONOMETHYLCYCLOPENTADIENYL RADICALS

R. S. Smith, L. F. DiMauro and T. A. Miller

Measurements have been made of the lifetimes of various vibrational levels of the lowest excited electronic state of the cyclopentadienyl, C_5H_5 , and methylcyclopentadienyl, $C_5H_4CH_3$, radicals. These measurements show a similar decrease in lifetime for each radical as the energy of the vibrational level is increased. These observations are consistent with a significant non-radiative decay route opening in the excited state.

Address of Smith and DiMauro: Department of Physics, Louisiana State University, Baton Rouge, LA 70803.

Address of Miller: Department of Chemistry, Ohio State University, Columbus, OH 43210.

RA4.

(9:16)

OPTICAL EMISSION STUDIES ON GRAPHITE IN A LASER/VAPORIZATION SUPERSONIC JET CLUSTER SOURCE

M. Anselmetti, R. S. Smith, E. Daykin, and L. F. DiMauro

C_2 Swann band emission ($d^3\Pi_g \rightarrow a^3\Pi_u$, 170 ns. lifetime) is observed in a supersonic free jet using a pulsed laser/vaporization source with a graphite target. In helium, Swann band emission is observed at distances of up to 15 nozzle diameters from the orifice and at times as long as 6 μ s after the vaporizing laser pulse. The emission studies are reported as a function of laser intensity, backing pressure, downstream distance, and delay times. Evidence supporting the continuous localized formation of excited C_2 molecules in the free jet via dissociative processes involving larger neutral and charged carbon clusters is presented, and the bearing of these results on the interpretation of cluster stability data is discussed.

Address: Department of Physics, Louisiana State University, Baton Rouge, LA 70803.

RA5.

(9:28)

LASER INDUCED FLUORESCENCE SPECTRA FROM PHOTOFRAGMENTS OF TOLUENE: A NEW ELECTRONIC TRANSITION OF C_2

L. J. VAN DE BURGT AND M. C. HEAVEN

The high fluence 193 nm photodissociation of toluene has been investigated in a free jet expansion. Laser induced fluorescence spectra of the products show a large number of resolved ro-vibronic bands in the range of 21,000 to 24,500 cm^{-1} . Many of these have been assigned to C_2 and C_3 . The C_2 is produced in metastable, electronically excited states, and a new band system originating from the $C^2\Sigma_u^+$ state has been observed. Two bands of this system, with origins at 22,347.0 and 22,462.5 cm^{-1} , show the simple P and R branch structure of a $\Sigma - \Sigma$ transition.

A preliminary rotational analysis yields an upper state rotational constant (for the band at 22,347 cm^{-1}) of 1.91 cm^{-1} , which is significantly larger than the constants for any of the previously characterized excited states.

The details of these experiments, and the results from a more extensive analysis of the spectra, will be presented.

Address of van de Burgt: Department of Chemistry, Northwestern University, Evanston, Illinois 60201.

Address of Heaven: Department of Chemistry, Emory University, Atlanta, Georgia 30322.

RA6.

(9:45)

LASER-INDUCED FLUORESCENCE FROM HCO AND DCO. NEW RESULTS

G.Rumbles, B.Stone, and E.K.C.Lee

Laser-induced fluorescence spectra have now been observed of several levels from both HCO and DCO. In addition to the spectrum of the $(0,9,0)$ level reported from HCO last year, we have now observed excitation and emission spectra from the following levels: $(0,11,0)$ and $(1,7,0)$ of HCO and $(0,11,0)$, $(0,13,0)$, and $(0,15,0)$ of DCO.

Emission to overtones of the CH stretch have been observed, revealing this vibration to be substantially anharmonic ($X_{11} = -165 \text{ cm}^{-1}$).

A computer simulation of the $(0,11,0)$ excitation spectrum of HCO has been performed, reliably predicting the rotational line positions. The anomalous intensity distribution is explained in terms of a K-type resonance, in which the linewidth is given by $\Delta\nu = 0.7 + (3 \times 10^{-5})J^2$ ($J + 1$)². In addition, some evidence exists of intensity borrowing due to Fermi resonance interaction.

B.M.Stone, M.Noble, and E.K.C.Lee, Chem. Phys. Lett., 118, 83 (1985)

Address of Rumbles: Dept. of Chemistry, University of California, Irvine, CA 92717

Address of Stone: Dept. of Chemistry, San Jose State University, San Jose, CA 95192

G.Rumbles and B.Stone deeply regret the demise of E.K.C.Lee

RA7.

(10:15)

EVIDENCE FOR A SECONDARY MINIMUM IN THE ArHCl POTENTIAL SURFACE FROM FAR INFRARED LASER/MICROWAVE DOUBLE RESONANCE SPECTROSCOPY OF THE LOWEST σ BENDING VIBRATION

R. L. ROBINSON, D.-H. GWO, D. RAY, AND R. J. SAYKALLY

The lowest σ bending vibration in the ArH³⁵Cl and ArH³⁷Cl van der Waals complexes have been measured near 24 cm^{-1} by Intracavity Far Infrared Laser Stark Spectroscopy and FIR/microwave double resonance. In conjunction with the calculations of Hutson,¹ the molecular constants provide strong evidence that the intermolecular potential energy surface contains two minima at the ArHCl and ArClH linear geometries.

1. J. M. Hutson, J. Chem. Soc. Faraday Trans. 2, 82, 1163 (1986).

Address of Robinson, Gwo, and Saykally: Department of Chemistry, University of California, Berkeley, CA 94720

Address of Ray: Joint Institute for Laboratory Astrophysics and Department of Chemistry, University of Colorado, Boulder, CO 80309

MEASUREMENT OF THE VAN DER WAALS STRETCHING VIBRATION IN ArHCl BY FAR INFRARED LASER/MICROWAVE DOUBLE RESONANCE SPECTROSCOPY

R. L. ROBINSON, D.-H. GWO, AND R. J. SAYKALLY

The first rotationally resolved spectrum of a van der Waals stretching vibration has been measured in the ArHCl molecular complex. Double resonance spectra have confirmed the assignment of the spectrum. The molecular constants are in good agreement with those of Hutson¹ for a double well potential and put the band origin at 32.4 cm^{-1} .

1. J.M. Huston, J. Chem. Soc. Faraday Trans. 2, 82, 1163 (1986).

Address of Robinson, Gwo, and Saykally: Department of Chemistry, University of California, Berkeley, CA 94720

FAR INFRARED OBSERVATIONS OF HYDROGEN-CONTAINING VAN DER WAALS MOLECULES

A.R.W. MCKELLAR

The intermolecular potential surfaces of the H_2 - rare gas pairs are perhaps the best characterized¹ of any triatomic system, thanks in part to previous mid-infrared spectra² of the H_2 -, and D_2 -rare gas Van der Waals molecules. These spectra accompany the various rotation-vibration transitions in the $v=1-0$ fundamentals of H_2 ($\approx 2.2 \mu\text{m}$) and D_2 ($\approx 3.2 \mu\text{m}$) and they are observed in low-temperature long-path absorption experiments. Similar spectra should accompany the pure rotational H_2 and D_2 lines in the far infrared (16 - 60 μm), and the first such experiments are the subject of this talk. The usual far infrared difficulties with exotic window materials, low source brightness, and low detector sensitivity make this work more difficult than that in the mid-infrared. The S(0) ($\approx 354 \text{ cm}^{-1}$) and S(1) ($\approx 587 \text{ cm}^{-1}$) spectra of H_2 -Ar have already been observed, and they should ultimately result in even better potential surfaces for these systems. The same regions in the spectrum of the dimer $(\text{H}_2)_2$ are also being studied, for the moment at 77 K (though lower temperature (15 K) experiments are also planned). These are of interest because of the observation of $(\text{H}_2)_2$ in Voyager spacecraft spectra of Jupiter and Saturn.³

¹ R. J. LeRoy and J. M. Hutson, J. Chem. Phys. 86, 837 (1987).

² A.R.W. McKellar, Faraday Discuss. Chem. Soc. 73, 89 (1982).

³ D. Gautier, A. Marten, J.P. Balateau, and G. Bachet, Can. J. Phys. 61, 1455 (1983); A.R.W. McKellar, Can. J. Phys. 62, 760 (1984); L. Frommhold, R. Samuelson, and G. Birnbaum, Astrophys. J. (Letters) 283, L79 (1984).

Address of McKellar: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada.

RA10.

(10:56)

RADICAL VAN DER WAALS MOLECULES

WAFAA FAWZY AND M. C. HEAVEN

Complexes consisting of a rare gas atom bound to a neutral free-radical provide prototype systems for the study of weak bonding interactions. In particular, when the radical possesses a permanent dipole moment, the relative importance of electrostatic interaction (dispersion forces) and chemical bonding (significant orbital overlap) can be qualitatively assessed.

Spectroscopic data (0.1 cm^{-1} resolution) for the vinoxy -Ar ($\text{C}_2\text{H}_3\text{O}-\text{Ar}$) complex has been partially analyzed to obtain structural information.³ The Ar is quite tightly bound, but the geometry is consistent with the dominance of electrostatic interactions. Studies of this complex at higher resolution, and attempts to observe the $\text{C}_2\text{H}_3\text{O}-\text{Ne}$ complex are currently in progress.

We are also examining the possibility of obtaining information about the weak bonding interaction by observing their effects on the spin-orbit coupling in triatomic adducts. The van der Waals complexes of SH and OH are useful model systems for this purpose, and we are searching for the electronic spectra of these adducts. A summary of the progress achieved in these studies will be presented.

Address of Fawzy and Heaven: Department of Chemistry, Emory University, Atlanta, GA 30322

RA11.

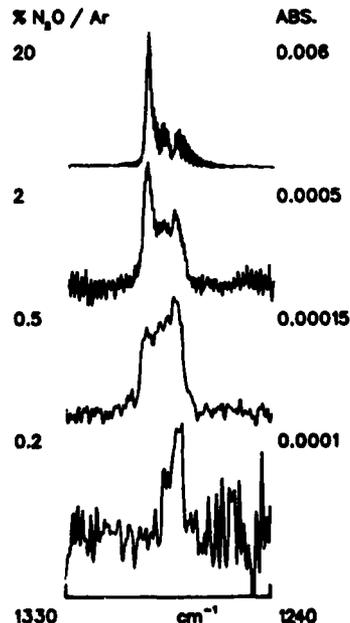
(11:13)

STRUCTURES OF N_2O DIMERS AND CLUSTERS FROM FTIR SPECTRA OF $\text{N}_2\text{O} / \text{Ar}$ SUPERSONIC EXPANSIONS

M. GAUTHIER AND P. A. HACKETT

In very dilute expansions, 0.2% N_2O in Ar, dimer bands at 1282 and 2228 cm^{-1} were observed corresponding to the ν_1 and ν_2 stretches of the monomer. As an example, the ν_1 region spectra are shown in the figure for various dilutions. In the dimer, the NO stretch frequency is reduced and the NN stretch frequency is increased consistent with a staggered parallel configuration with the O atoms towards the centre. The dimer band at 2228 cm^{-1} is shifted +5 cm^{-1} while the $\text{Ar}-\text{N}_2\text{O}$ complex band origin shift is only +0.1509 cm^{-1} .

"Cluster bands" (we have no means of determining the cluster size) corresponding to 6 bands of the monomer were readily observed in rich mixtures, ~2-100% N_2O , at 1165, 1296, 2246, 2467, 2578, and 3506 cm^{-1} . For all three bands $2\nu_1$, ν_1 , and ν_2 , observed here and in the crystal², the cluster shift is larger and in the same direction. In SF_6-Ar_n clusters³, a sharp peak appeared in the linewidth against size for clusters around $n=14$ which suggested a phase change. Such a peak was not observed here. Rather, the linewidths decreased monotonically with richer mixtures (larger clusters) suggesting a structure getting more and more rigid, as in the high pressure range of the SF_6 work. (N_2O)_n linewidths were in the range 2-3 cm^{-1} . Helium as a carrier gas gave the same results although clustering was more pronounced in Argon.



- 1) J.Hodge, G.D.Hayman, T.R.Dyke and B.R.Howard, J.Chem.Soc., Faraday Trans. 2, 82, 1137 (1986).
- 2) A.Anderson and T.S.Sun, Chem.Phys.Letters, 8, 537 (1971).
- 3) D.Eichenauer and R.J.LeRoy, Phys.Rev.Letters, 57, 2920 (1986).

Address : Laser Chemistry Group, National Research Council, Ottawa, Canada, K1A 0R6.

RA12.

(11:30)

DETERMINATION OF THE STRUCTURE OF OCS CO₂S. E. NOVICK, R. D. SUENRAM, AND F. J. LOVAS

The rotational spectrum of the weakly bound complex OCS CO₂ has been measured using a pulsed beam Fourier transform microwave spectrometer.

The rotational constants of the major isotopic form are A=4454.590 MHz, B=1517.743 MHz, and C=1129.707 MHz.

The molecule is planar; its structure is analogous to the C_{2h} structure of (CO₂)₂ as determined from high resolution infrared spectroscopy by R. E. Miller et al.¹ Analysis of the spectrum, structure, and dipole moment will be presented.

¹R. E. Miller, K. W. Jucks, Z. S. Huang, G. T. Fraser, A. S. Pine, and W. J. Lafferty. Talk presented, this Symposium.

Address of Novick: Department of Chemistry, Wesleyan University, Middletown, CT, 06457.

Address of Suenram and Lovas: Molecular Spectroscopy Division, National Bureau of Standards, Gaithersburg, MD 20899.

RA13.

(11:47)

BROADBAND, TIME RESOLVED INFRARED ABSORBANCE SPECTROSCOPY OF TRANSIENT SPECIES

M. A. Young and G. C. Pimentel

A spectrometer that is capable of simultaneously probing a broad infrared spectral range, from 1360cm⁻¹ to 800cm⁻¹, while achieving a time resolution of one nanosecond has been constructed. The overall scheme is based on the work of Sorokin et.al.¹. The IR probe source is generated by stimulated Raman scattering in a metal vapor. Broadband signal collection is facilitated by an infrared multichannel analyzer. The highest resolution obtained thus far is approximately .5cm⁻¹.

The IR absorption spectra of several gas phase radicals have been obtained and the recombination rate constants have been determined. The application of the technique to the excited singlet and triplet states of molecules will be discussed.

¹P.P. Sorokin et. al., IBM J. of Res. and Dev., 23(5), 556, (1979).

Address of Young and Pimentel: Dept. of Chemistry, Univ. of Calif., Berkeley, Cal. 94720.

RB2.

(9:03)

CALCULATION OF HIGH RESOLUTION SPECTRA OF H₂O BY MEANS OF PARTICLES-ON-A-SPHERE MODEL

DAVID M. LEITNER, PABLO VILLARREAL, GERARDO DELGADO-BARRIO, JOHN E. HUNTER III, GRIGORY A. NATANSON, and R. STEPHEN BERRY

The adiabatic separation of high-frequency stretching modes from bending and rotational motions in H₂O leads naturally to the particles-on-a-sphere model.¹ Compared with the previous calculations, this model has been extended to include the interaction of stretching modes. In addition, an algorithm for the evaluation of intensities using an electric dipole moment function² measured in the bisector frame has been developed.

A new potential, suitable for representing both the region around the equilibrium point and regions of much longer O-H distances and other bond angles, has been generated from available potentials and is used to generate energy levels and eigenfunctions for rotation-vibration states over a wide range of energy.

¹G.A. Natanson, G.S. Ezra, G. Delgado-Barrio, R.S. Berry, (a) J. Chem. Phys., 81, 3400 (1984); (b) J. Chem. Phys., 84, 2035 (1986).

²B.J. Rosenberg, W.C. Ermler, I. Shavitt, J. Chem. Phys., 65, 4072 (1976).

Address of Leitner, Hunter, and Berry: Department of Chemistry, The University of Chicago, Chicago, Illinois 60637.

Address of Villarreal and Delgado-Barrio: Institute de Estructura de la Materia, C.S.I.C., Serano, 119, Madrid-6, Spain.

Address of Natanson: Department of Chemistry, Northwestern University, Evanston, Illinois 60201.

RB3.

(9:15)

CALCULATION OF THE ROTATIONAL PART OF THE INVERSE OF THE FOUR DIMENSIONAL GENERALIZED TENSOR OF INERTIA OF MOLECULES WITH ONE LARGE-AMPLITUDE INTERNAL MOTION

VIKTOR SZALAY

Maintaining the physical ideas of a previous work¹ but using a new mathematical formulation, a simpler method is suggested for calculating the rotational part of the inverse of the four dimensional generalized tensor of inertia of molecules with one large-amplitude internal motion. The theory includes molecules whose large-amplitude internal motion produces an internal angular velocity of variable direction.

¹V. Szalay, J. Mol. Spectrosc. 103, 13(1983).

Address of Szalay: Herzberg Institute of Astrophysics, National Research Council of Canada, Ottawa, Canada K1A 0R6

RB4.

(9:32)

INTERNAL ROTATION IN METHYL SILANE: A SEMIRIGID BENDER ANALYSIS

R. ESCRIBANO AND P.R. BUNKER

There is a wealth of data on the energy levels associated with overall rotation and torsion of methyl silane;¹ so far these data have been analyzed by the principal axis method (PAM) or the internal axis method (IAM).^{1,2} We will present here the application of the semirigid bender hamiltonian in an attempt to interpret the existing data by using a few molecular parameters that have a straightforward physical meaning (bond lengths and bond angles, and their variations with the internal rotation angle), plus the usual potential energy expansion coefficients.

¹N. Moazzen-Ahmadi, I. Ozier and H. Jagannath, J. Mol. Spectrosc. 119, 299 (1986) and references therein.

²E. Hirota, J. Mol. Spectrosc. 43, 36 (1972).

Address: Herzberg Institute of Astrophysics, National Research Council, Ottawa, K1A 0R6 Canada

RB5.

(9:49)

ABSOLUTE INFRARED INTENSITIES OF FUNDAMENTAL MODES OF H₂O. CALCULATIONS AND EXPERIMENTS WITH MATRIX-ISOLATED H₂O¹M. SZCZESNIAK,² K. KUBULAT, RODNEY J. BARTLETT AND WILLIS B. PERSON

Ab initio MO calculations of infrared intensities of H₂O predict infrared intensities for the fundamental modes that differ considerably from the reported experimental values. Even when these calculations are made at the highest level of theory (the dipole derivatives were calculated with a very large basis set, using fourth order MBPT and CCSD + T(CCSD)) the predictions for the intensity of ν_1 and for ν_2 are too high, compared with experimental values. This discrepancy has inspired us to measure relative intensities of these fundamental modes for samples of H₂O isolated in Ar, N₂ and CO matrices. The results will be discussed critically in an attempt to resolve the discrepancy between theory and experiment for this important test molecule.

¹ Work done at the Department of Chemistry, University of Florida, Gainesville, FL 32611.

Work supported by NIH Grant No. GM32988 and by CRDEC Contract No. DAA15-85-C0034.

² On leave 1986-7 from the Institute of Physics, Polish Academy of Science, 02668 Warsaw, Poland.

Address of Szczesniak, Kubulat, Bartlett and Person: Department of Chemistry, University of Florida, Gainesville, FL 32611.

RB6.

(10:06)

AB INITIO PREDICTIONS AND INTERPRETATION OF INFRARED SPECTRA OF DERIVATIVES OF H_3PO ¹

JOZEF S. KWIATKOWSKI,² K. KUBULAT, RODNEY J. BARTLETT AND WILLIS B. PERSON

Ab initio MO calculations of infrared spectra are presented for H_3PO and related phosphorous-containing compounds. The calculated spectra are compared with experimental spectra from several laboratories; agreement is generally satisfactory. The calculated force constants, normal coordinates, and atomic polar tensors are examined and interpreted to indicate the structural explanations for the observed frequencies and intensities of the bands in the spectrum.

¹ Work done at the Department of Chemistry, University of Florida, Gainesville, FL 32611. Supported by CRDEC Contract No. DAA15-85-C0034.

² On leave 1985-6 from Institute of Physics, N. Copernicus University, 87-100 Torun, Poland.

Address of Kwiatkowski, Kubulat, Bartlett and Person: Department of Chemistry, University of Florida, Gainesville, FL 32611.

RB7.

(10:35)

THE INFLUENCE OF PRESSURE ON THE NH_3 ν_3 FUNDAMENTAL ABSORPTION SPECTRUM

STEVEN A. HENCK AND KEVIN K. LEHMANN

We will present data on the lineshape of ν_3 absorption lines in the pressure regime where two lines from a given inversion doublet become overlapped. From the lineshape as a function of pressure, we will determine the degree to which optical coherence is transferred across the inversion doublet.

Address of Henck and Lehmann: Department of Chemistry, Princeton University
Princeton N.J. 08544

RB8.

(10:47)

ROTATIONAL AND VIBRATIONAL ANALYSIS OF
THE 2 N-H STRETCH REGION OF AMMONIA (6700 cm^{-1})

Stephen L. Coy and Kevin K. Lehmann

Rotational analysis of the vibrational bands in the 2 N-H stretch region of ammonia is in progress with the assistance of new microwave-optical double resonance data, new BOMEM FTIR spectral data at room temperature and at dry ice, and the results of resonance RAMAN experiments. The rotational analysis makes it possible to identify the character of observed vibrational bands. The vibrational band data is leading to a local-mode anharmonic force field for ammonia. Current progress will be reported.

Address of Coy: Harvard U. Dept. of Chemistry, 12 Oxford Street, Cambridge, MA 02138

Address of Lehmann: Princeton U. Dept. of Chemistry, Princeton, NJ 08544

RB9.

(10:59)

Assignment of the $\nu_1+\nu_2$ and $\nu_2+\nu_3$ bands of the high resolution $^{14}\text{NH}_3$ FTS absorption spectra

N. Tu, G. Guelachvili, and K. N. Rao

The Fourier transform absorption spectra of NH_3 with a resolution of 0.005 cm^{-1} were recorded at Laboratoire D'Infrarouge of Universite de Paris-Sud. The assignment of the $\nu_1+\nu_2$ and $\nu_2+\nu_3$ bands of NH_3 has been carried out for the J value as high as 13. The inversion-rotational energy levels of the ground states of $^{14}\text{NH}_3$ has been calculated. These energy levels are compared with the best previous work⁽¹⁾ which shows an agreement within 0.001 cm^{-1} .

(1) S. Urban, Romola D'Cunha, K. Narahari Rao, and D. Papousek, Canad. J. Phys. **62**, 1775-1791 (1984).

Address: The Ohio State University, Department of Physics, Columbus, OH 43210

RB10.

(11:16)

SUBMILLIMETER LASER STARK SPECTROSCOPY OF ND_3

R. L. BHATTACHARJEE, G. R. SUDHAKARAN, J. C. SARKER, AND L. H. JOHNSTON

A Laser Stark spectrum has been observed for fully deuterated ammonia ($^{14}\text{ND}_3$) with the $195\mu\text{m}$ line of the DCN laser up to Stark fields of about 58000 V/cm . The rotation-inversion spectra were taken for both parallel and perpendicular polarizations and three distinct families, one above the laser line and two below the laser line, were observed. Tentative identification of the family above the laser line is $a \leftarrow s$, $J_K = 5_1 \leftarrow 4_1$ and those below the laser frequency are $s \leftarrow a$, $J_K = 5_4 \leftarrow 4_4$, $5_3 \leftarrow 4_3$.

Address of the authors: Department of Physics, University of Idaho, Moscow, ID 83843

RB11.

(11:33)

INFRARED SPECTRA OF UNSTABLE MOLECULES USING THE BURST OF

GAS TECHNIQUE. T. C. DEVORE, T. R. BURKHOLDER, AND T. N.

GALLAHER.

A simple, home built combination chemical reactor infrared cell has been coupled with FT-IR to produce the infrared spectra of a variety of molecules which are unstable under ambient conditions. The chemical reactions used and the infrared spectra obtained for the TiF_4 , AlCl_3 , Al_2Cl_6 , $\text{SO}(\text{OCN})_2$, KOCN , and the $\text{K}_2(\text{OCN})_2$ gaseous molecules will be discussed.

Address of DeVore, Burkholder and Gallaher: Department of Chemistry, James Madison University, Harrisonburg, VA 22807.

SUBPICOSECOND AMMONIA PHOTODISSOCIATION RATES AS DETERMINED BY RESONANCE ROTATIONAL HYPER-RAMAN SCATTERING

Y.C. Chung, J.L. Roebber and L.D. Ziegler

We report the first rotationally and vibrationally resolved resonance hyper-Raman (RHR) spectra. When blue light is focused in NH_3 (or ND_3) at pressures of 1 to 5 atm, a Raman spectrum in the ultraviolet is observed. The frequency of this visible incident radiation is exactly half the transition frequency of the $\bar{X}(A_1') \rightarrow \bar{A}(A_2'')$ electronic excitation. The corresponding absorption is diffuse owing to the rapid unity quantum yield photodissociation to NH_2 and H. The analysis of the observed rotationally resolved RHR spectra reveal rotationally and vibrationally dependent subpicosecond excited state lifetimes. This technique is the two-photon analog to our linear resonance rotational Raman analysis.^{1,2} The quantum specific lifetimes determined by the RHR studies are interpreted in terms of the subpicosecond ammonia photodissociation mechanism.

1. L.D. Ziegler, J. Chem. Phys., 86, 1703 (1987).
2. L.D. Ziegler, J. Chem. Phys., 84, 6013 (1986).

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RC1.

(8:30)

A REVIEW OF RECENT EXPERIMENTAL STUDIES OF THE INFRARED SPECTRA OF SOLID HYDROGEN ISOTOPES

James R. Gaines

Using a high resolution Fourier transform spectrophotometer (BOMEM), my colleagues consisting of Sang Young Lee, Tae Won Noh, Sung-Ik Lee, John P. Golben, and Robert D. McMichael have obtained the spectra of solid and liquid HD from 400 cm^{-1} and $12,000\text{ cm}^{-1}$. In the solid phase, the intensities of several zero-phonon transitions and those of the accompanying phonon branches were measured. In the liquid phase, the zero-phonon transitions were slightly weaker than those of solid phase.

In addition, the first and second vibrational overtone transitions of molecular D_2 in the solid and liquid phases have been observed between 400 cm^{-1} and 9500 cm^{-1} . The transparent solid crystals were grown from ortho, para and normal D_2 to a length 2.6 cm inside the cell. The pure vibration-rotation transitions in the first overtone of the solid phase were accompanied by the phonon branches. In the liquid phase, the zero-phonon transitions were slightly weaker than those of the solid phase. The much weaker lines of the second overtone were also observed by increasing the signal to noise ratio using several methods. The two sets of experiments will be discussed in this talk.

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RC2.

(9:05)

ABSORPTION SPECTRA OF SOLID MOLECULAR HYDROGEN IN THE FIRST OVERTONE REGION¹

S. PADDI REDDY, G. VARGHESE AND R. D. G. PRASAD

Solid hydrogen crystals of both para and normal species were grown in a glass cell 6.4 cm long and 1.0 cm in diameter using liquid helium cryogenics apparatus. Their infrared absorption spectra were recorded in the first overtone region $8000 - 9400\text{ cm}^{-1}$. The absolute intensities of several zero phonon transitions of the type $Q_2(J)$, $Q_1(J) + Q_1(J)$, $S_2(J)$, $Q_2(J) + S_0(J)$, $Q_1(J) + S_1(J)$, $S_2(J) + S_0(J)$ and $S_1(J) + S_1(J)$ and those of the accompanying phonon branches Q_R and S_R were measured. The observed spectra clearly demonstrate that there is no contribution to the intensity of the pure overtone Q_R phonon branch from isotropic electron overlap induction mechanism. This is in striking contrast to the observations in the fundamental band of either solid² or gaseous³ hydrogen.

¹Supported by NSERC Grant No. A-2440.

²H. P. Gush, W. F. J. Hare, E. J. Allen and H. L. Welsh, Can. J. Phys. **38**, 176 (1960).

³S. P. Reddy, G. Varghese and R. D. G. Prasad, Phys. Rev. A **15**, 975 (1977).

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Address of Prasad: Ranchi University, Ranchi, India.

RC3.

(9:22)

COLLISIONAL INTERFERENCE IN THE PURE ROTATIONAL SPECTRUM OF HD PERTURBED BY FOREIGN GASES

P.G. DRAKOPOULOS AND G.C. TABISZ

The rotational transitions R(0), R(1), R(2) and R(3) have been studied at 0.06 cm^{-1} resolution in pure HD and in mixtures with all inert gases at 295K. The permanent dipole moment of HD was found to be 8.83(28), 7.94(2), 7.88(3) and 8.43(10), in units of 10^{-18} debye, for R(0) to R(3), respectively. There is interference between the allowed and collision-induced transitions characterized by an interference parameter which varies as the ratio of the average induced moment to the allowed moment. It showed a systematic dependence, both in magnitude and sign, on the perturber polarizability and on the rotational quantum number J. The sign of the overlap induced moment could be specified. The line shapes were generally found to be symmetrical although there was some asymmetry evident for light perturbers and for the R(1) profile. Comparison with earlier experiments and theory of line shapes and intensities will be made.

Address of Drakopoulos and Tabisz: Department of Physics, University of Manitoba, Winnipeg, Manitoba, Canada, R3T 2N2.

RC4.

(9:39)

COLLISION INDUCED ABSORPTION AS A FUNCTION OF TEMPERATURE FOR N_2 , CO_2 , and SF_6

M. E. THOMAS and M. J. LINEVSKY

High pressure transmission measurements of N_2 , CO_2 , and SF_6 are taken using a BOMEM DA3.02 vacuum spectrometer. A 30.5 cm long cell capable of 68 atm maximum pressure and of temperatures from 295 to 500 K is used in the experiment. The entire optical path is under vacuum. The spectral range covered is from 1800 to 5000 cm^{-1} .

Measurements of the integrated intensity on the collision induced absorption (CIA) of the fundamental vibration band of N_2 are obtained as a function of temperature. Our results and others^{1,2,3} are compared to the theory by Van Kranendonk.⁴ An excellent fit is obtained from 77K to 500K.

Integrated intensities are also obtained for the $2\nu_1$ and $\nu_2 + \nu_3$ CIA bands of pure CO_2 and mixtures with N_2 . These bands are strongly influenced by N_2 .³

CIA contributions to the intensity of the infrared allowed $3\nu_3$ band was observed and at the highest pressure (21.1 atm), accounted for approximately 50% of the integrated intensity. The CIA contributions fall off rapidly with increasing temperature.

1. N. I. Moshalenko, Yu A. Ibin, S. M. Parzhin, and L. V. Rodionov, *Izvestiya Atmos. Ocean Phys.* **15** 632-637 (1979).

2. M. M. Shapiro and H. P. Gush, *Can. J. Phys.* **44**, p. 949 (1966).

3. D. T. Sheng and G. E. Ewing, *J. Chem. Phys.* **55**, p. 5425 (1971).

4. J. Van Kranendonk, *Physica*, **24**, p. 347-362 (1958).

The Johns Hopkins University, Applied Physics Laboratory, Laurel, MD. 20707

RC5.

(9:56)

RAMAN SPECTRA OF SOLID MOLECULAR NITROGEN

G. Guelachvili(*) (**), G. Pangilinan(**), K. Narahari Rao(**), R. Sooryakumar(**) and R. H. Tipping(***) .

Due to the simpler geometrical arrangement, the theoretical interpretation of molecular interactions may be easier in the lattice than in the gas phase. In the case of the nitrogen molecule, the structure of the solid at normal pressure is known. A phase transition occurs at a temperature $T_{ph} = 35.6K$. The crystal is cubic ($\alpha-N_2$) for $T < T_{ph}$, and hexagonal ($\beta-N_2$) for $T > T_{ph}$.

This paper reports preliminary results of a Raman scattering study on single crystal N_2 . The experiment is specifically designed to investigate the effect of the above structural phase transition on the molecular and phonon excitations. The crystal (4x2x2 cm) is grown in a cryostat where the temperature is servo controlled over a large domain by appropriate heating of a flow of gaseous helium. The spectra are excited with a krypton laser and the scattered beam recorded with a spectral resolution equal to about 1 cm^{-1} .

The crystal cell, the optical system to enhance the signal to noise ratio and the growth technique are also described.

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(***) Dept. of Physics and Astronomy, The University of Alabama, Tuscaloosa Alabama, 35487, USA.

RC6.

(10:25)

RESONANCE RAMAN EXCITATION PROFILES OF Cu(II) CHELATED 1,4-DIHYDROXYANTHRAQUINONE

T.S. KOCH AND R.P. RAVA

Resonance Raman excitation profiles have been obtained for the fundamental vibration bands of Cu(II) chelates of 1,4-dihydroxyanthraquinone in ethanol. Under the experimental conditions these complexes exhibit a textbook Franck-Condon absorption spectra for a displaced harmonic oscillator. Yet the resonance Raman excitation profiles show that the primary resonance enhanced bands do not follow calculated Franck-Condon excitation profiles. The sensitivity of the excitation profiles to perturbations including vibronic coupling, Duschinsky rotations and Raman interference effects will be discussed.

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RC7.

(10:42)

RESONANCE RAMAN INTERFERENCE IN LINEAR POLYENES

I. SZTAINBUCH AND G. E. LEROI

In centrosymmetric chromophores, such as linear polyenes, approximately half of the electronic excited state manifold is inaccessible from the ground state by conventional absorption spectroscopy because of parity selection rules. However, the presence of such "hidden" excited states can sometimes be inferred from preresonance Raman excitation profiles. As the excitation radiation is tuned through the appropriate energy range, vibronic coupling between the state of interest and nearby "allowed" electronic states will produce interference effects in the ground state scattering intensity. Thrash, et al.¹ used this method to determine the approximate origin of the lowest lying excited gerade single state (¹A_g^{*}) of β-carotene, preresonant with the neighboring higher-energy ¹B_u^{*} state.

We have reexamined the preresonance Raman excitation profile of β-carotene, using improved instrumentation and a careful statistical analysis. Excitation was supplied by an Ar⁺-pumped tunable dye laser in the wavelength regions covered by rhodamine 560 and coumarin 540. The excitation spectrum was determined point-by-point from the ratio of the scattered intensity of the β-carotene C=C stretch (1525 cm⁻¹) to that of the cyclohexane solvent made at 1450 cm⁻¹. The interference pattern observed previously is generally confirmed; however, inherent experimental uncertainties limit the inferences which may be drawn from such excitation profiles. The technique has been applied to other linear polyenes, and results for all systems investigated to date will be described.

¹R. J. Thrash, H. L.-B. Fang and G. E. Leroi, J. Chem. Phys. **67**, 5930 (1977).

Address of Sztainbuch and Leroi: Department of Chemistry, Michigan State University, East Lansing, Michigan, 48824.

RC8.

(10:59)

RAMAN TRACE SCATTERING INTENSITY PARAMETERS FOR HYDROCARBONS

K. M. GOUGH and W. F. MURPHY

In a recent study of vibrational properties of deuterium isolated CH bonds in *n*-alkanes,¹ it was found that when the proton can occupy more than one position (e.g., propane CHD₂CD₂CD₃, and cyclohexane-*d*₁₁), the relative Raman intensity ratios for the CH stretching bands varied significantly from values predicted on the basis of widely held assumptions regarding the intensity behavior and relative conformer abundance. To resolve this difficulty, we have measured the absolute Raman trace scattering cross sections of selected isotopomers of various alkanes. The observed cross sections for a set of isotopomers were fit in terms of isotopically invariant intensity parameters and, for isotopomers where more than one conformer can coexist, the relative conformer abundance.

In an initial study of ethane, we verified that the over-all fit of the integrated cross sections was not significantly affected by neglecting the anharmonic contributions to the vibrational force field and the intensity. In subsequent studies of propane and cyclohexane, we have found that the reason for the anomalous intensity ratios is the unexpectedly large variation (~15%) in the intensity parameter $\partial\bar{\alpha}/\partial r_{CH}$ for the in-plane and out-of-plane methyl CH bonds in propane and for the axial and equatorial CH bonds in cyclohexane. The relative conformer abundance result is consistent with a random distribution of the proton among available sites, to within the accuracy of our experiment.

We also find that there is a significant variation in the parameter $\partial\bar{\alpha}/\partial r_{CC}$ for the three alkanes studied. These results call into serious question the assumption of the transferability of such parameters when estimating Raman trace scattering cross sections.

¹R. G. Snyder *et al.*, J. Chem. Phys. **81**, 5352-5361 (1984).

²K. M. Gough and W. F. Murphy, J. Chem. Phys. **85**, 4290-4296 (1986).

Address: Division of Chemistry, National Research Council of Canada, Ottawa, Canada K1A 0R6.

RC9.

(11:16)

RECENT MEASUREMENTS OF ABSOLUTE INFRARED ABSORPTION INTENSITIES OF LIQUIDS

John E. Bertie, H. Harke, K. Ahmed, and H. H. Eysel

Our attenuated total reflection method for measuring absolute infrared absorption intensities of liquids as the real and imaginary refractive indices and, hence, the real and imaginary dielectric constants has been developed and applied. Recent results for liquid water and alcohols will be presented and related to molecular properties.

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Address of Eysel : Institut für Anorganische Chemie, der Universität Heidelberg, Heidelberg, West Germany.

RC10.

(11:33)

INFRARED SPECTRA OF ADSORBATES ON ELECTRODE SURFACES

Mark W. Severson and P. P. Schmidt

We present in situ infrared spectra of triatomic ions such as azide and tetrahedral ions such as sulfate adsorbed on a platinum metal electrode. To describe these systems, we use a simple model in which the interaction between the adsorbate and the surface is represented by a sum of two-center potential functions. Two effects contribute to the shifts in the vibrational frequencies upon adsorption. The first arises from the changes in the intramolecular force constants; these changes are due to the distorted geometry of the adsorbed molecule. The second effect is due to the force constants which arise from the intermolecular potential energy functions. The model is used to obtain information on the adsorbate orientation, and on the relative strength of the surface-adsorbate interaction.

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RC11.

(11:50)

SURFACE ENHANCED RAMAN STUDY OF BENZIDINE ON Ag ELECTRODE: AN INTERPRETATION FOR DIFFERENT ADSORPTION CONFIGURATIONS AT VARIOUS APPLIED VOLTAGES

GUOHAI LIU AND GUOZHEN WU

The surface enhanced Raman spectra of benzidine in the Ag sol and on the Ag electrode at different applied voltages are reported. These spectra are compared with those in the crystalline form and in the dimethyl sulfoxide solution with the group theoretical analysis. It is interpreted that in the Ag sol and on the Ag electrode with voltage larger than -0.2 V (with respect to the standard Calomel electrode) the benzidine molecule is adsorbed perpendicularly with one of its two amino groups attached on the Ag surface. While the applied voltages on the Ag surface are less than -0.4 V both of its amino groups are adsorbed on the Ag surface with the flat configuration. The adsorption mechanism for these two configurations is also proposed in the report.

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RC12.

(12:02)

FREEZING OF A DIATOMIC FLUID

SHERWIN J. SINGER, JOHN D. MCCOY, AND DAVID CHANDLER

The freezing transition in a fluid of diatomic molecules is described by expressing the liquid-solid free energy difference as a functional of the inhomogeneous density $\rho(r)$. The theory predicts how the aspherical nature of the molecules affects the freezing density, as well as the translational and orientational distribution of molecules in the solid. This talk presents theoretical results for a "hard dumbbell" model for diatomics, the simplest model that captures the effect of packing among aspherical molecules.

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Address of McCoy and Chandler: Department of Chemistry, University of California, Berkeley, CA, 94720.

RD1.

(8:30)

THE TRANSFORMATION BETWEEN INTERNAL DISPLACEMENT COORDINATES AND NORMAL COORDINATES OF POLYATOMIC MOLECULES

H.C. HSIEH, W.C. ERMILER AND E.R. MALINOWSKI

Potential energy surfaces in normal coordinates, derived from the transformation of each grid point of the ab initio internal coordinate surfaces, and those regenerated in small increments using the force constants obtained from fitting the same surface in internal displacement coordinates are compared. The effect of the propagation of the standard deviations in force constants in internal coordinate expansions to the normal coordinate surface and, subsequently, the spectroscopic constants, frequencies, and transition intensities of polyatomic molecules is analyzed. Deviations are obtained using a Monte Carlo method under a Gaussian probability distribution. This procedure results in the most dependable error analysis.

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RD2.

(8:42)

VIBRATIONAL-ROTATIONAL ANALYSIS OF AB INITIO POTENTIAL ENERGY SURFACES FOR SYMMETRIC-TOP MOLECULES: APPLICATION TO AMMONIA ISOTOPOMERS

L.O. HARGISS AND W.C. ERMILER

An ab initio potential energy surface for ammonia has been used to calculate vibrational-rotational spectroscopic constants. A complete quartic Taylor series fit in both internal and normal coordinates was derived. Spectroscopic constants were calculated for deuterated isotopomers using normal coordinate force constants, equilibrium geometries, and normal mode eigenvectors within the framework of second-order perturbation theory. Anharmonic spectroscopic constants for ammonia compare favorably with other ab initio calculations. Normal mode force constants are in reasonable agreement with empirically obtained values.

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RD3.

(8:54)

HIGH QUALITY CH₂ POTENTIAL ENERGY SURFACES

DONALD C. COMEAU AND ISAIAH SHAVITT

Multireference CI potential energy surfaces for the ³B₁ and ¹A₁ states of CH₂ are being computed using a very large basis set and a complete valence space reference set. These surfaces will allow the calculation of accurate minimum-energy geometries, vibrational energy levels, and the zero-point vibrational contributions to the singlet-triplet splitting. They should also facilitate improved accuracy in the determination of the singlet-triplet splitting from the experimental laser magnetic resonance data.¹

¹A. R. W. McKellar, P. R. Bunker, T. J. Sears, K. M. Evenson, R. J. Saykally and S. R. Langhoff, *J. Chem. Phys.* 79, 5251 (1983).

Address: Department of Chemistry, The Ohio State University, Columbus, Ohio 43210.

RD4.

(9:16)

STEREOMUTATION OF METHANE

MELANIE J. M. PEPPER AND ISAAH SHAVITT

A possible transition state for the stereomutation of methane has been proposed by Schleyer.¹ The structure is of C_s symmetry, with the four hydrogen atoms forming an isosceles trapezoid in a plane. Energy gradient calculations have been performed at the SCF and MCSCF levels to determine the optimum transition state geometry and vibrational frequencies. Single reference and multireference CI calculations have been performed on the optimum C_s structure and on the CH_3 dissociation fragment, thus allowing comparison of the energies of dissociation and stereomutation.

¹P. von R. Schleyer, private communication.

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RD5.

(9:33)

STRUCTURES AND ROTATIONAL CONSTANTS OF C_4O AND C_5O D. W. EWING

The microwave spectrum of C_3O has recently been observed in interstellar space¹. This has led to speculation that C_2O ,² and perhaps C_4O , may also be present in the interstellar medium². The goal of the present calculations is to predict rotational constants accurately enough to allow a search for these rotational lines in the interstellar medium.

Molecular orbital calculations have been performed at the Hartree-Fock (HF) and post-HF (MP3) levels using Pople's 6-31G* basis set³. Results for C_4O and C_5O are compared to previous work on C_3O ⁴. Trends in structure, electronic configuration, and rotational constants are discussed.

¹H. E. Matthews, W. M. Irvine, P. Friberg, R. D. Brown, and P. D. Godfrey, *Nature* **310**, 125 (1984).

²B. E. Turner, private communication.

³P. C. Hariharan and J. A. Pople, *Chem. Phys. Lett.* **66**, 217 (1972).

⁴R. D. Brown and E. H. N. Rice, *J. Am. Chem. Soc.* **106**, 6475 (1984).

Address: Department of Chemistry, John Carroll University, Cleveland, Ohio 44118

RD6.

(9:45)

STUDY OF THE EFFECTS OF COMPLEX SCALING ON THE CONVERGENCE OF BASIS SET EXPANSION TECHNIQUES AS APPLIED TO THE PROPAGATION OF WAVEPACKETS.

Steven D. Parker and C. William McCurdy, Jr.

Convergence properties of wavepacket propagation in a finite basis are seen to be improved by complex scaling of the underlying coordinates or parameters of the basis set. The resulting matrix representation of the hamiltonian in the $EXP(-iHt/h)$ is complex symmetric and therefore nonhermitian. Two systems are examined. The first system is a model, one-dimensional, Gaussian wavepacket propagated through free space. The second is the propagation of a probability distribution function for a one-electron atom which is closely related to the frequency-dependent polarizability and therefore the photoionization cross section.

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RD7.

(10:15)

PHOTOIONIZATION CROSS SECTIONS FOR SF₆ BY THE COMPLEX BASIS FUNCTION METHODChin-hui Yu, Russell M. Pitzer and C. William McCurdy

In the complex-basis-function method the photoionization cross section is computed from a representation of the resolvent of the molecular electronic Hamiltonian in a basis set consisting of a mixture of real and complex Gaussian basis functions. Previously, this method has been successfully applied in a nonlinear system, the bending vibrational mode of CO₂, as well as in linear molecules, such as H₂, N₂ and CO₂. In this work, the application of this *ab initio* method is extended to SF₆. Results of calculations of the photoionization cross sections for forming the A²T_{1U} ionic state are reported. An interesting feature is the near-threshold resonance in the 5t_{1U}→ka_{1g} partial channel. A comparison is made with available experimental data.

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RD8.

(10:32)

RESTRICTED HARTREE-FOCK WAVEFUNCTIONS AND EXCITATION ENERGIES OF ALKOXY RADICALS

Stella M. Sung and Russell M. Pitzer

Ab initio calculations have been performed that generate the restricted Hartree-Fock wavefunctions and the transition energies for the ground state and lower excited states of the hydroxy (OH), methoxy (CH₃O), ethoxy (C₂H₅O), isopropoxy (C₃H₇O), and vinyloxy (C₂H₃O) radicals. These theoretical results are compared to results obtained from laser excitation spectra that were recorded in a supersonic free jet expansion at low temperature for these radicals (Foster, Hsu, Damo, Liu, Kung, and Miller). These calculations attempt to resolve uncertainties in the assignment of the ground and excited states from the spectroscopic results for the vinyloxy and isopropoxy radicals.

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RD9.

(10:49)

POTENTIAL CURVES AND AVOIDED CROSSINGS FOR THE CuF MOLECULE

Nora M. Wallace and Russell M. Pitzer

Although the CuF spectrum has been assigned, there is more analysis to be done of the interaction of states and their behavior as the molecule dissociates. Potential energy curves have been computed from configuration interaction calculations that include spin-orbit coupling. Core and spin-orbit potentials were used on both atoms along with an optimized (6s5p5d/4s5p), (6s3p5d/2s3p) basis set. Calculations of the energy of the ground state and several excited states were carried out at a number of internuclear distances. Symmetry was used to make the Hamiltonian matrix real and avoid complex arithmetic. The predominant spatial symmetry of each state was tracked in order to examine spin-orbit induced avoided crossings. The ground state and lower excited states show the expected ionic behavior at the equilibrium internuclear distance and the expected covalent behavior at infinite internuclear distance.

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RD10.

(11:06)

ELECTRONIC STRUCTURE OF URANOCENE

Agnes Chang and Russell M. Pitzer

Uranocene, $U(C_8H_8)_2$, is a D_{8h} actinide analog of ferrocene. Valence electronic wavefunctions are computed using core and spin-orbit potentials provided by P. Christiansen. Double-zeta level basis sets are used in the valence regions. The structural features investigated are the barrier to ring rotation and the out-of-plane position of the H atoms. Excited states correspond both to excitations among the 5f-like orbitals and to ligand-to-metal transitions. A number of positive ion states were investigated for comparison with the photoelectron spectrum. All calculations were done with configuration-interaction (including spin-orbit) wavefunctions of modest length.

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RD11.

(11:23)

THEORETICAL STUDIES OF DIVALENT VANADIUM IN A MAGNESIUM FLUORIDE HOST

N. W. Winter and R. M. Pitzer

Divalent vanadium substituted into weak field fluoride crystals is an example of a 'phonon-terminated' four-level laser with the emission terminating on vibrationally excited levels of the ground electronic state. Laser action in vanadium-doped magnesium fluoride ($MgF_2:V^{+2}$) at a wavelength of $1.12 \mu m$ (8915 cm^{-1}) was reported by Johnson et. al.¹ as early as 1966. In an extensive experimental study of the optical properties of $MgF_2:V^{+2}$, Moulton et. al.² discovered an unfavorably strong excited-state-absorption (ESA) transition which overlapped the ${}^4T_2 \rightarrow {}^4A_2$ laser transition. We have carried out configuration interaction electronic structure calculations on the ground and excited states of $MgF_2:V^{+2}$ in order to better understand the nature of the ground and excited state absorption. These theoretical studies represent the most accurate *ab initio* calculation of the optical spectrum of an ion/host system to date. The calculated position of the zero-phonon line corresponding to the origin of the ${}^4T_2(B_2)$ absorption band was found to be in error by only 2-3%. Similar accuracy was obtained for the peak of the ${}^4A_2 \rightarrow {}^4T_2$ absorption. As determined from the calculated potential energy curves, the predicted peak of the ${}^4T_2 \rightarrow {}^4A_2$ emission at 9195 cm^{-1} is in error by only -275 cm^{-1} (3%), which is consistent with the magnitude of the agreement for the zero-phonon line, but opposite in sign. The energies for the ESA transitions from the ${}^4T_2(B_2)$ state to the crystal field split components of the ${}^4T_{1a}$ and ${}^4T_{1b}$ excited states have been calculated and will be discussed.

¹L. F. Johnson, J. H. Guggenheim, and R. A. Thomas, *Phonon Terminated Optical Masers*, Phys. Rev. 149, 179 (1966); L. F. Johnson and J. H. Guggenheim, *Phonon Terminated Coherent Emission from V^{+2} Ions in MgF_2* , J. Appl. Phys. 38, 4837 (1967).

²1981 Laser Program Annual Report, Lawrence Livermore National Laboratory, Livermore, Calif., UCRL-50021-81 (1982), p 7-94; 1982 Laser Program Annual Report, Lawrence Livermore National Laboratory, Livermore, Calif., UCRL-50021-82 (1983), p 7-78.

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This work was performed under the auspices of the United States Department of Energy by the Lawrence Livermore National Laboratory under contract W-7405-Eng-48

RD12.

(11:40)

THEORETICAL PREDICTION OF CONDUCTIVITY IN DOPED AND UNDOPED POLYMERS

G.P. Das and J.E. Mark

With the discovery of polyacetylene as a commercially viable electrical conductor (when doped with suitable materials), many other polymers became of interest with regard to their conductivity properties. As far as theory is concerned, the traditional Extended Huckel Theory (EHT) and the more recent Valence Effective Hamiltonian (VEH) approach have been applied to study the conductivity bands, their widths, and the band-gaps. On this basis, one can make predictions on the nature of the conductivity. We present here calculations on the polymer systems polybenzobisoxazole (PBO) and polybenzobisthiazole (PBT) using the VEH formalism. We also present total energy calculations based on an approximate *ab-initio* theory to supplement the above calculations.

Address: Polymer Research Center, University of Cincinnati, Cincinnati, OH 45221

RD13.

(11:57)

AB INITIO HIGHER DERIVATIVES: CUBIC FORCE FIELDS FOR CF_3H , $CClF_2H$, AND CCl_3H AND A QUARTIC FORCE FIELD FOR CH_4

Jeffrey F. Gaw and Nicholas C. Handy

Self-consistent-field (SCF) analytic third derivatives with respect to nuclear perturbations for both closed¹ and open² shell molecules can now be routinely calculated for molecules of spectroscopic interest. In this talk, two such studies will be reported.

Recently, the interactions of the stretching and bending motions of the isolated CH chromophores in CF_3H , $CClF_2H$, CCl_3H , and CD_3H have attracted much experimental attention³. We have evaluated the SCF cubic force field analytically for these systems using a variety of cartesian gaussian basis sets. The interpretation of both the experimental and theoretical data will be discussed.

The best fit of experimental data to obtain an anharmonic force field for CH_4 has been performed by Gray and Robiette⁴. In their analysis, a single quartic force constant (f_{rrrr}) and full cubic force field were utilized. We have calculated the complete *ab initio* quartic force field. Fourth derivatives were obtained from finite differences of analytic third derivatives. The resulting *ab initio* anharmonic constants will be presented and discussed.

Finally, recent progress in the analytic evaluation of SCF fourth derivatives will be presented.

¹J. F. Gaw, Y. Yamaguchi, H. F. Schaefer, and N. C. Handy, J. Chem. Phys. **85**, 5132 (1986).

²J. F. Gaw, Y. Yamaguchi, R. B. Remington, Y. Osamura, and H. F. Schaefer, Chem. Phys. **109**, 237 (1986).

³See, for example, J. Segall, R. N. Zare, H. R. Dubal, M. Lewerenz, and M. Quack, J. Chem. Phys. **86**, 634 (1987).

⁴D. L. Gray and A. G. Robiette, Molec. Phys. **37**, 1901 (1979).

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RE6.

(4:29)

ROTATIONAL SPECTRUM AND BENDING POTENTIAL OF LITHIUM HYDROXIDE

D. McNAUGHTON, L. M. TACK, B. KLEIBÖMER, AND P. D. GODFREY

Some 29 microwave transitions have been measured in the high-temperature vapour of LiOH, ranging up to $J = 5$, including lines from the isotopomers ${}^7\text{Li}{}^{16}\text{OH}$, ${}^7\text{Li}{}^{16}\text{OD}$ in both ground and excited bending states, and ${}^7\text{Li}{}^{18}\text{OH}$ in the vibrational ground state only. An analysis based on the semirigid bender model of vibration-rotation interaction has been used to investigate the form of the bending potential, and to measure the semirigidity parameters that show the variation in the bond lengths that accompanies the large amplitude motion. In this analysis, use was made of earlier radiofrequency l -doubling transition data¹. The molecule was found to be linear in its equilibrium configuration, with an essentially harmonic bending potential. The experimentally derived quadratic semirigidity parameters were found to agree to within 5% with those from an *ab initio* calculation at the MP3/6-311G** level.

¹S. M. Freund, Ph.D. Thesis, Harvard University, (1970).

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RE7.

(4:46)

EXTENDED ANALYSIS OF THE π BENDING VIBRATION-ROTATION SPECTRUM OF ArHCl BY INTRACAVITY FAR INFRARED LASER/MICROWAVE DOUBLE RESONANCE SPECTROSCOPY

R.L. ROBINSON, D. RAY, D.-H. GWO, AND R. J. SAYKALLY

The lowest π bending state in ArHCl has been more fully characterized using far infrared laser/microwave double resonance spectroscopy. This analysis includes a reassignment of the far infrared spectrum of ArH³⁵Cl previously reported by Ray *et al.* and Marshall *et al.*, as well as an analysis of the ArH³⁷Cl spectrum. The following new molecular constants have been determined for the π state in ArH³⁵Cl: $\nu = 1018.6861(3)$ GHz, $B = 1740.9(1)$ MHz, $q_1 = -49.1(3)$ MHz, $\nu = .2603(2)$ D, $eqQ_{aa} = 5.6(2.7)$ MHz, and $eqQ_{bb} - eqQ_{cc} = -73.2(2.7)$ MHz; and for ArH³⁷Cl: $\nu = 1018.4700(3)$ MHz, $B = 1691.4(2)$ MHz, $q_1 = -47.0(3)$ MHz, $\nu = .2606(1)$ D, $eqQ_{aa} = 4.0(1.8)$ MHz, and $eqQ_{bb} - eqQ_{cc} = -57.3(1.8)$ MHz. The new value of the rotational constant gives much better agreement with the value calculated by Hutson¹ from the M5 double minimum potential surface than the previous value. Thus with the recently reported spectrum of the Σ bending vibration of ArHCl² this analysis provides further strong support for a double minimum character in the van der Waals surface. In addition, the powerful combination of the double resonance technique, to assign complicated spectra, with the sensitive intracavity spectroscopic technique has been demonstrated.

1. J.M. Hutson, J. Chem. Soc. Faraday Trans. 2, **82**, 1163 (1986).

2. R.L. Robinson, D.-H. Gwo, D. Ray, and R.J. Saykally, J. Chem. Phys. **86**, in press (1987).

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Address of Ray: Joint Institute for Laboratory Astrophysics and Department of Chemistry, University of Colorado, Boulder, CO 80309

RES.

(4:58)

DIODE LASER VELOCITY MODULATION SPECTROSCOPY OF CARBANIONS: THE C-C STRETCHING ;MODE OF ACETYLIDE (C_2H^-)

M. GRUEBELE, M. POLAK, AND R.J. SAYKALLY

Ten lines in the C-C stretching vibration of C_2H^- have been assigned and fit with a linear molecule Hamiltonian. The molecular constants are remarkably close to those of neutral C_2H , except for the vibrational band origin, which lies 87 cm^{-1} below the neutral radical band origin. This is in keeping with the expected lower electron density between the carbons in C_2H^- .

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FA1.

(8:30)

STATE SELECTIVE PHOTOFRAGMENTATION OF ICl-Ne VAN DER WAALS COMPLEXES

Janet C. Drobits and Marsha I. Lester

The vibrational predissociation dynamics of ICl-Ne van der Waals complexes has been investigated for a series of vibrational levels in the $A(^2\Pi_1)$ state manifold. Visible laser excitation prepares the complexes in selected rovibrational levels in the A state. Coupling of the vibrational excitation, initially localized in the ICl bond, to the weak van der Waals bond results in predissociation of the complex. Fragmentation proceeds with the loss of one or two quanta of ICl vibrational energy. The nascent rotational/vibrational distribution is probed by excitation of the ICl A state photofragments to an ion pair state. The product state distribution reflects the dominant features of the reaction pathway and provides an important key to understanding the reaction mechanism.

By initially populating different vibrational levels in the complex, the energetics and lifetime of the predissociation can be selectively altered. Detailed product state distributions will be presented for dissociation of ICl-Ne from A state vibrational levels with predissociation lifetimes ranging from nanoseconds¹ to a few picoseconds. Analysis of results will be discussed in the context of statistical theories of photodissociation and inelastic scattering theories.

¹J.C. Drobits, J.M. Skene and M.I. Lester, *J. Chem. Phys.* **84**, 2896 (1986).

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FA2.

(8:47)

RESONANT PHOTOIONIZATION SPECTROSCOPY OF REFRACTORY METAL-RARE GAS COMPLEXES

John M. Gardner and Marsha I. Lester

The weakly attractive interatomic potential between a refractory metal and a rare gas atom is explored by direct spectroscopic access of rovibronic levels in the AlAr van der Waals complex. Mass-resolved resonance-enhanced multiphoton ionization is used to probe the spectral region about the $Al\ ^2S_{1/2} - ^2P_{1/2}$ transition. A vibrational progression in the AlAr $^2\Sigma^+$ state is identified on the AlAr⁺ mass channel. Lower limits for binding energies in the X $^2\Pi_{1/2}$ and B $^2\Sigma^+$ states are found to be 133 and 373 cm^{-1} , respectively. Results are compared to earlier work on NaAr.

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FA3.

(9:04)

OPTOTHERMAL CORRELATION SPECTROSCOPY OF VAN DER WAALS COMPLEXES

G.T. FRASER AND A.S. PINE

The characteristics of an optothermal molecular beam spectrometer constructed at the National Bureau of Standards for the high-resolution study of van der Waals complexes will be discussed. As with similar instruments developed by Miller and coworkers¹, a cryogenic bolometer detects an adiabatically expanded helium beam seeded with an active species which is excited by a tunable color-center laser in a nearly orthogonal geometry for sub-Doppler resolution. The F-center laser scanning is actively servo-controlled for precision linearity, reproducibility and calibration. Data processing correlation techniques to enhance the signal-to-noise ratio and eliminate false peaks arising from random thermal spikes generated by microcrystallization of the seed gas condensate on the bolometer substrate will be discussed. Applications of the instrument to several van der Waals species such as the carbon dioxide dimer and trimer will be given.

1. Z.S. Huang, K.W. Jucks and R.E. Miller, J. Chem. Phys. **85**, 3338 (1986) and references therein.

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FA4.

(9:21)

SUB-DOPPLER MOLECULAR BEAM SPECTROSCOPY OF
TWO COMBINATION BANDS OF THE CARBON DIOXIDE DIMERR.E. MILLER, K.W. JUCKS, Z.S. HUANG, G.T. FRASER, A.S. PINE, and W.J. LAFFERTY

Two bands of the carbon dioxide dimer have been obtained using optothermal molecular-beam spectrometers at both NBS and the Univ. of NC. The spectra were obtained in a CO₂:He beam with the CO₂ concentration ranging from 2 to 13 % and driving pressures ranging from 7 to 2 atmospheres. The rotational temperature was about 2 K. The observed line widths were instrumentally limited and were less than 20 MHz. These bands are associated with the monomer bands, $\nu_1 + \nu_3$ and $2\nu_2^0 + \nu_3$, at 3714 and 3612 cm⁻¹.

Both bands are hybrid a- and b-type bands with the a- and b-type transitions having nearly equal intensities. The lower frequency band was readily assigned with transitions originating in energy levels as high as $K_a''=4$ and $J''=12$. The observed wavenumbers were fit using a Watson Hamiltonian with a overall standard deviation of ± 0.00008 cm⁻¹. The higher frequency band is perturbed and, at this time, line assignment is proceeding with the aid of ground state combination differences obtained from the unperturbed band.

Transitions with K_c odd are missing from the observed spectra. Since all the nuclei in the dimer have zero nuclear spin and the observed inertial defect is small, this implies that the complex must have C_{2h} symmetry. The A, B, and C rotational constants, obtained by fitting ground state combination differences from both bands are: 0.3002864(42), 0.0535994(13), and 0.0453409(12) cm⁻¹ respectively. The observed inertial defect is 1.172 amu A². If the C=O distance is assumed to be unchanged from that of the monomer, the C...C distance in the dimer is 3.602 Å and the C...CO angle is 58.4°.

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FA5.

(9:38)

SUB-DOPPLER INFRARED SPECTRUM OF THE CARBON DIOXIDE TRIMER

G.T. FRASER, A.S. PINE, W.J. LAFFERTY AND R.E. MILLER

A spectrum of the carbon dioxide trimer van der Waals species has been recorded near 3613 cm^{-1} at sub-Doppler resolution using an optothermal (bolometer-detected) molecular-beam color-center laser spectrometer. The trimer transitions are distinguished from the dimer lines in the same region by their pressure and concentration dependence. The trimer spectrum is that of an oblate symmetric top with missing $K = 3N \pm 1$ subbands due to the vanishing statistical weights arising from the off-axis zero nuclear spin ^{12}C and ^{16}O atoms. A precise fit of the low temperature ($T \sim 1.3\text{ K}$) spectrum is obtained with a planar, cyclic structure of C_{3h} symmetry with $B'' = 0.0398088(47)\text{ cm}^{-1}$ and a carbon-carbon spacing of $4.0382(3)\text{ \AA}$. No tunneling or perturbations are observed. The angle of the monomer axes away from a tangential D_{3h} structure is estimated to be $\sim 43^\circ$ from considerations of the electrostatic quadrupole-quadrupole potential and the van der Waals radii.

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FA6.

(9:55)

SUB-DOPPLER RESOLUTION INFRARED SPECTROSCOPY OF $\text{H}_2\text{-HF}$

K. W. JUCKS AND R. E. MILLER

The optothermal detection method has been used to obtain sub-doppler resolution infrared spectra for the HF stretching vibration of $\text{H}_2\text{-HF}$. At the highest resolution obtained in this study, the homogeneous broadening associated with the finite lifetime of the excited vibrational state (27 ns) is just observable. Infrared Stark spectra have also been recorded from which the electric dipole moments in the ground (1.428D) and excited (1.512D) vibrational states have been determined. These results clearly show that the HF monomer unit undergoes wide amplitude bending in both the ground and vibrationally excited states and that the bending angle decreases upon vibrational excitation.

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FA7.

(10:10)

ROTATIONAL PERTURBATIONS IN THE INFRARED SPECTRA OF SEVERAL BINARY COMPLEXES

Z. S. HUANG, K. W. JUCKS AND R. E. MILLER

High resolution near infrared spectra have been recorded for a number of binary complexes using laser-molecular beam methods. Several of these spectra show perturbations resulting from either Coriolis or anharmonic coupling between the state of interest and other (nearly degenerate) vibrational states of the molecule. Examples of these will be shown for $(\text{N}_2\text{O})_2$, OC-HF , NCCN-HF and $(\text{HCN})_2$. Several interesting correlations between the strength of the coupling and the width of the observed transitions (due to vibrational relaxation) will be discussed.

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FAB.

(10:40)

INFRARED SPECTROSCOPY AND VIBRATIONAL PREDISSOCIATION OF $(\text{HCN})_2$ AND $(\text{HCN})_3$

K. W. JUCKS AND R. E. MILLER

The rovibrational spectra of both the free (ν_1) and hydrogen bonded (ν_2) C-H stretches of $(\text{HCN})_2$ have been measured using the molecular beam bolometric detection technique. In the case of the free stretch, the transitions have instrument limited linewidths, indicating a very long vibrational predissociation lifetime. For the hydrogen bonded stretch, however, lifetime broadening of the transitions is observed. In the ν_2 band, many of the transitions associated with low J' states are significantly broader than those associated with higher J' . This effect is believed to result from perturbations due to Coriolis or anharmonic couplings with nearby vibrational states. In addition, several bands associated with higher clusters have been observed. One of these has been assigned as the free C-H stretch of a linear conformer of $(\text{HCN})_3$. Due to the small coupling between the free C-H stretch and the van der Waals bond, transitions associated with this band are found to be narrow. An additional band is observed to the red of the hydrogen bonded dimer band and is believed to correspond to the hydrogen bonded linear trimer stretches. In this case, however, no rotational fine structure is resolved. One final band is observed midway between the free and hydrogen bonded dimer bands. This spectrum is clearly associated with an oblate symmetric top and is most likely the cyclic conformer of the trimer. Further work is underway in an attempt to verify this latter assignment and to ensure that this band is not due to a higher order cluster.

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FA9.

(10:57)

THE STRUCTURE OF $(\text{N}_2\text{O})_2$ FROM SUB-DOPPLER RESOLUTION NEAR INFRARED SPECTROSCOPY

Z. S. HUANG AND R. E. MILLER

A rotationally resolved near infrared spectrum of $(\text{N}_2\text{O})_2$ has been obtained, corresponding to the $\nu_1 + \nu_3$ band of the N_2O monomer using the molecular beam optothermal detection technique. The spectrum has been assigned to an asymmetric rigid rotor structure with both A- and B-type transitions present. From the nuclear spin statistics, arising from the nitrogen nuclei, and the ground state rotational constants, the structure of the dimer has been determined to be planar (offset anti-parallel) with C_{2h} symmetry. This is similar to the structure determined previously for $(\text{CO}_2)_2$. Local perturbations are observed in $K = 0$ and 1 of the excited vibrational state. Further work is underway to completely assign the spectrum in an effort to understand the pattern and origin of the local perturbation. It is interesting to note that the dimer spectrum is shifted slightly to the red of the monomer origin while the larger clusters are observed to be blue shifted.

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FA10.

(11:14)

INFRARED VIBRATION-ROTATION SPECTRUM OF ACETYLENE TRIMER

DIANA PRICHARD, J. S. MUENTER, AND B. J. HOWARD

The infrared spectrum of acetylene trimer has been recorded in the three micron wavelength region by observing direct absorption of color center laser radiation by a pulsed molecular beam. The rotational structure of this band was that of a planar symmetric top. The B rotational constant is 1885.8 MHz which fixes the distance between the centers of mass of each monomer and the center of mass of the trimer at 2.513 Å. This monomer separation is consistent with a trimer geometry of D_{3h} or C_{3v} symmetry having atoms of adjacent monomer units close to van der Waals contact.

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FA11.

(11:29)

INFRARED VIBRATION-ROTATION SPECTRUM OF ARGON-ACETYLENE

DIANA PRICHARD, J. S. MUENTER, AND B. J. HOWARD

The infrared spectrum of argon-acetylene has been recorded in the three micron wavelength region by observing direct absorption of color center laser radiation by a pulsed molecular beam. Thirty transitions in the P_{P_1} , P_{Q_1} , R_{Q_0} , R_{R_0} , R_{Q_1} , and R_{R_1} bands of a perpendicular transition have been assigned. The origin of this Ar-HCCH vibrational transition is about 0.3 cm^{-1} lower in energy than the ν_1 monomer origin. The rotational structure yields values for A and B-C which are consistent with an earlier radio frequency spectrum of Ar-HCCH. However, $(B+C)/2$ from the infrared spectrum is much smaller than the earlier prediction. Argon-acetylene exhibits an extremely large inertial defect, which explains the poor prediction based on the radio frequency spectrum.

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FA12.

(11:44)

INFRARED SPECTRA OF ACETYLENE CLUSTER MOLECULES

DIANA PRICHARD, J. S. MUENTER, AND B. J. HOWARD

The infrared spectrum of what is believed to be acetylene dimer has been recorded in the three micron wavelength region by observing direct absorption of color center laser radiation by a pulsed molecular beam. Over 100 individual transitions have been measured in a very dense portion of the infrared spectrum of acetylene polymers. These transitions lie in a range of about three wavenumbers centered at the $P(4)$ line of the $\nu_{2,3}$ band of the monomer. Efforts to assign these transitions are currently in progress. Other segments of the three micron spectrum also show absorptions from acetylene polymers, and these will be discussed qualitatively.

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FB1.

(8:30)

VIBRATION-ROTATIONAL INTENSITIES FOR DIATOMIC MOLECULES OF ASTROPHYSICAL INTEREST: THE ISOVALENT MOLECULES CO, CS, SiO AND SiS

R. H. TIPPING, A. LOPEZ PINEIRO, AND C. CHACKERIAN, JR.

Vibration-rotational dipole moment matrix elements and Einstein A coefficients have been calculated for a group of isovalent molecules of astrophysical interest. The wavefunctions used were obtained by a direct numerical integration of the radial Schrodinger equation with an RKR potential-energy function. The dipole-moment functions were represented by Pade' approximants which have the correct theoretical long-range dependence on the inter-nuclear separation. The coefficients in these expressions were obtained for CO, CS and SiO from experimental intensity data and/or ab initio calculations. For SiS for which only the permanent dipole moment is known, we estimated the intensities from the systematic trends found for the other three isovalent molecules.

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FB2.

(8:42)

DEUTERIUM HYPERFINE STRUCTURE IN INTERSTELLAR CYCLOPROPENYLIDENE-d₁ (C₃HD)

M. B. BELL, H. E. MATTHEWS, P. A. FELDMAN, L. W. AVERY, J. K. G. WATSON, W. M. IRVINE, AND S. C. MADDEN

The rotational transition $1_{10} - 1_{01}$ of the isotope C₃HD of the ubiquitous interstellar ring molecule C₃H₂ was recently identified¹ in the interstellar molecular cloud TMC-1. New observations on a different sub-cloud of TMC-1 show fully resolved deuterium hyperfine structure of the same transition. The values of the deuterium quadrupole coupling parameters $eQ_0q_{zz} = 188$ kHz, $\eta = 0.053$, appear very normal for this unique molecule. The relative intensities indicate departures from local thermal equilibrium which will be discussed.

¹ M. B. Bell, P. A. Feldman, H. E. Matthews, and L. W. Avery, Ap. J. (Letters) 311, L99 (1986).

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FB3.

(8:49)

THE INTENSITIES OF HCN OVERTONE TRANSITIONS FROM 12,600 - 18,400 cm^{-1}

A. M. SMITH and K. K. LEHMANN

The absolute intensities of twelve visible overtone bands of HCN have been determined using intracavity photoacoustic detection and a long pathlength absorption cell.

The relative intensities of nine of these weak overtone bands (from 14,600-18,400 cm^{-1}) were obtained by using intracavity photoacoustic detection. The absolute intensity of the (0,0,5) band, obtained previously using a multipass cell with an optical pathlength \times pressure of about 34 km-torr¹, was used to calibrate the photoacoustic response, and thus to obtain the absolute intensities for eight more HCN overtone bands.

The absolute intensities of three HCN overtone bands between 12,600-13,800 cm^{-1} were measured using a multipass cell. Optical pathlengths \times pressure from 10 km-torr to 15 km-torr were used for these three bands.

The approximate band origins^{2,3} in cm^{-1} , the band labels (CN, bend, CH), and the intensities in cm^2/mol are:

12636, (0,0,4), 154(3)	14654, (4,0,2), 8.0(4)	16674, (2,0,4), 1.7(1)
15552, (0,0,5), 17.5(4)	14670, (1,0,4), 7.2(4)	16640, (5,0,2), 0.40(4)
17550, (1,0,5), 13.9(4)	13702, (2,0,3), 3.1(2)	15710, (3,0,3), 0.05(1)
12658, (3,0,2), 8.5(1.1)	18377, (0,0,6), 2.4(2)	16164, (0,1 ¹ ,5), 0.047(8)

¹A. M. Smith, K. K. Lehmann, and W. K. Klemperer, J. Chem. Phys. **85**, 4958-4965 (1986).

²K. K. Lehmann, PhD thesis, Harvard University, 1983.

³A. E. Douglas and D. Sharma, J. Chem. Phys. **21**, 448.458 (1952).

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Address of Lehmann: Frick Chemical Laboratories, Princeton University, Princeton, New Jersey 08544.

FB4.

(9:06)

DIPOLE MOMENTS OF VIBRATIONAL OVERTONE LEVELS OF HCN

J.A. Dodd, A.M. Smith and W. Klemperer

Dipole moments for the (0,0,5) (15,552 cm^{-1}) and (1,0,5) (17,550 cm^{-1}) vibrational overtone levels of HCN have been determined: $\mu_{005} = 3.141 \pm 0.004$ D and $\mu_{105} = 3.159 \pm 0.011$ D. The experiment uses an applied DC electric field, in which the Stark plates form two walls of a resonant acoustical cell. The apparatus is placed within the cavity of a narrowband, visible dye laser, and is rotated to measure both parallel and perpendicular DC Stark shifts. The photoacoustic signal is detected with a microphone attached to the ground plate. Observed ground state Stark shifts provide an internal calibration of the applied field.

The experimental dipole moments will be compared to ab initio and semi-empirical predictions for the dipole moment function.

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FB5.

(9:18)

PHOSPHINE IN THE 5 μM OBSERVATION WINDOW OF JUPITER :
LINE STRENGTHS, H_2 - AND He - BROADENED WIDTHS

N. Lacombe, A. Lévy, G. Tarrago, G. Poussigue and G. Guelachvili

Laboratory spectra of pure, hydrogen- and helium-broadened phosphine were recorded, near 5 μm , using high resolution Fourier transform spectrometer (apodized resolution 0.0054 cm^{-1}).

The lines under study belong mainly to the $\nu_2 + \nu_4$ transition. A number of lines pertaining to the neighbouring $2\nu_2$ and $2\nu_4$ (\perp and \parallel) bands were also analyzed.

A first series of spectra, of pure phosphine under low pressure (~ 0.3 Torr) at 296 and 180 K, was used for vibration-rotation analysis and line strength measurements.

A second set, consisting of hydrogen- and helium-broadened spectra (total pressure ~ 120 Torr) at temperatures ranging from 170 to 296 K, yielded collisional line widths along with their temperature dependence.

The true broadening coefficients and line strengths were directly derived from the measured values of the apparent width and peak transmission of the recorded lines. For this purpose, correction tables were previously built up by convolving the instrument function of the interferometer with a series of synthetic Voigt lines of given strengths and lorentzian widths.

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FB6.

(9:35)

MODELLING OF PHOSPHINE ABSORPTION IN THE 2050-2150 CM^{-1} JOVIAN WINDOW

G. Tarrago, G. Poussigue, N. Lacombe, A. Levy and G. Guelachvili

In order to account for the PH_3 features observed in the Jovian spectrum at 5 μm , the three interacting bands $2\nu_2$, $\nu_2 + \nu_4$ and $2\nu_4$ contributing to the absorption in the window 2050-2150 cm^{-1} were analyzed from laboratory spectra*. The parallel and perpendicular components of the $2\nu_4$ (strongly overlapped at room temperature by the red wings of ν_1 and ν_3) were assigned for the first time, from a low temperature spectrum.

The three bands were analyzed within a triad Hamiltonian model where the strong Coriolis couplings among the upper vibrational states were explicitly included in the energy matrix before diagonalization.

The series of required computing programs was similar to that previously set up for the analysis of CH_3D at 6-10 μm (1).

The energy and intensity parameters presently derived were used for modelling the absorption frequencies and intensities in the window. All transitions predicted with line strengths above the lower limit of $4 \cdot 10^{-25} \text{ cm/molecule}$ were taken into account.

* For experimental details, see the paper on PH_3 by Lacombe *et al.*

(1) G. Tarrago and M. Delaveau, J. Mol. Spectrosc. 119, 418-425 (1986).

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FB7.

(9:47)

CLOSED-FORM EXPRESSIONS FOR LOW-TEMPERATURE ROTATIONAL PARTITION FUNCTIONS

ROBIN S. McDOWELL

Modern non-equilibrium spectroscopic cooling techniques, as well as possible astrophysical applications, make it necessary to evaluate rotational partition functions, Q_r , at temperatures low enough for the usual closed-form expressions to become inaccurate, but still high enough for direct summation to be cumbersome. We will demonstrate that analytic expressions for Q_r can be derived that provide much greater accuracy at all temperatures, and extend the range of validity to significantly lower temperatures. For spherical-top XY_n molecules, such a formula is

$$Q_r = \sigma^* \pi^{1/2} e^{\alpha/4} \alpha^{-3/2} (1 + \delta) (1 + 15D/4\alpha B),$$

where $\alpha = hcB/kT$ and $\sigma^* = (2I_Y + 1)^n / \sigma$ (I_Y = nuclear spin of the Y nuclei, σ = classical symmetry number). Here the first four factors are the usual high-temperature quantum-mechanical partition function, accurate to within 1% for $\alpha < 0.2$ (i.e., for $T > 38$ K for CH_4). The factor in δ corrects for low-temperature quantum effects, and the last factor accounts for centrifugal distortion. For CH_4 , $\delta = \frac{1}{2} \exp(2.31 - 1.10/\alpha)$, and this formula is accurate to within 0.002% for $58 < T \leq 500$ K, and to within 0.1% down to 18 K. For octahedral hexafluorides, $\delta = -\exp(-0.35 - 0.60/\alpha)$, and Q_r is accurate to within 0.002% down to 1.2 K for SF_6 .

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FB8.

(10:10)

LOW TEMPERATURE MEASUREMENTS OF PLANETARY GASES

S. NADLER, J. J. HILLMAN, AND D. E. JENNINGS

A low temperature absorption cell has been used to obtain spectra between 100 and 300 Kelvin of planetary gases. These spectra were recorded with our Doppler-limited diode laser spectrometer and with the 1-m FTS located at the McMath Solar Telescope at the National Solar Observatory, operated at 0.0025 cm^{-1} resolution. We undertook an investigation of the spectrum of ethane, propane, and ethylene under H_2 -broadened conditions at temperatures appropriate to the outer planets. A modified confocal étalon facilitated precise measurement of line positions. We will discuss these experiments, the basic results, and the implications for planetary modeling.

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FB9.

(10:22)

INFRARED LINE INTENSITIES OF C10 FROM HIGH RESOLUTION FOURIER TRANSFORM SPECTROSCOPY^{*}J. J. HILLMAN, T. KOSTIUK, J. L. FARIS, AND M. J. MUMMA

⁻¹Infrared line intensities of C10 in the fundamental rotation-vibration (1-0) band near 850 cm^{-1} are inferred from a (Herman-Wallis type) rotation-vibration interaction analysis of Fourier transform spectra. These data were recorded with the one-meter FTS located at the McMath solar telescope at the National Solar Observatory. The FTS was used in the double-pass mode to produce an unapodized spectral resolution of 0.0025 cm^{-1} .

We will present details of the experiment, results of the analysis, comparison with previous works, and a discussion of the intrinsic sensitivity of the technique for the determination of vibrational band intensities.

^{*} This research is supported, in part, by the NASA Upper Atmosphere Program.

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FB10.

(10:39)

INTENSITIES AND H₂-BROADENED HALF-WIDTHS OF GERMANE LINES AROUND 4.7 μm AT TEMPERATURES RELEVANT TO JUPITER'S ATMOSPHERE†

P. VARANASI and S. CHUDAMANI

Absolute intensities and H₂-broadened half-widths of R(0) and R(1) of ⁷²GeH₄ have been measured at 119.5, 150.3, 199.0, 250.0, and 296.0 K using a tunable diode laser and the sweep integration technique. The combined intensity of the ν₃ bands of all of the five isotopic species of GeH₄ as well as that of the Q-branches alone have been measured independently at 294 K using the Wilson-Wells-Penner-Weber technique.

†Supported by the Planetary Atmospheres Branch of the Solar System Exploration Division of NASA under Grant-in-Aid No. 33-015-139.

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FB11.

(10:56)

MEASUREMENT OF N₂-BROADENED LINE WIDTHS OF CO AT LOW TEMPERATURES†

S. CHUDAMANI, P. VARANASI, and S. KAPUR

Analyses of CO spectra observed in the atmospheres of Earth and Titan require N₂-broadened line width data at low temperatures. We have, therefore, measured the N₂-broadened half-widths of several lines between P(1) and P(15) in the fundamental band of ¹²C¹⁶O at 100, 150, 200, 250, and 298 K in our laboratory. Employing a tunable diode laser spectrometer and the sweep-integration technique, the line widths (cm⁻¹atm⁻¹) have been found to vary with temperature according to the empirical power law:

$$\gamma^o \sim T^{-n}$$

with $n = 0.746 \pm 0.016$.

†Supported by the Planetary Atmospheres Branch of the Solar System Exploration Division of NASA under Grant-in-Aid No. 33-015-139.

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FB12.

(11:13)

WATER VAPOR CONTINUUM BEYOND 8 MICRONS†**P. VARANASI, S. CHUDAMANI AND S. KAPUR**

The continuum absorption by water vapor beyond 8 μm plays an important role in atmospheric remote sensing and climate analysis research studies. The nature of this absorption spectrum and its dependence upon atmospheric temperature, pressure and humidity have been examined in our laboratory. A brief discussion of the existing theoretical models is presented along with new experimental data.

†Supported by The Atmospheric Sciences Division of NSF under Grant No. ATM 83-17115.

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FB13.

(11:30)

LINE POSITION MEASUREMENTS OF N₂O AT ELEVATED TEMPERATURES**MARK P. ESPLIN AND WILLIAM M. BAROWY**

Spectra of N₂O in the 1100 to 1400 cm^{-1} region have been measured using a 3.5 m path high temperature absorption cell and the AFGL high resolution interferometer. The spectra were taken at a resolution of 0.006 cm^{-1} , and at temperatures of 300K, 473K, and 800K. The pressure of the N₂O samples ranged from 1 to 15 torr, and were of natural isotopic abundance. There are two main band systems in the 1100 to 1400 cm^{-1} region of N₂O, the 10⁰ ← 00⁰ and the 02⁰ ← 00⁰ bands and their associated "hot bands." Effective rotation-vibration constants which predict the position of spectral lines for both types of bands will be presented.

This work was supported by the Air Force Office of Scientific Research as part of AFGL Task 2310G1.

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LINE STRENGTHS OF THE ν_2 AND ν_4 BANDS OF METHANE**M. LOÛTE, J. C. HILICO, and L. R. BROWN**

Absolute line strengths of the ν_2 and ν_4 bands of $^{12}\text{CH}_4$ in the 1000-1800 cm^{-1} region have been measured from high resolution spectra recorded on the F.T. spectrometer at Kitt Peak.

871 well isolated lines of these two bands, up to $J = 21$, have been selected and analyzed simultaneously in a dyad scheme (548 lines for ν_4 and 323 lines for ν_2).

This analysis has required a second order dipole moment development involving 7 parameters. The relative standard deviation is around 3 %, in agreement with the experimental precision. It will be shown that individual deviations are evenly distributed in the two bands and between allowed and forbidden lines.

The complete spectrum up to $J = 23$ has been calculated including about 11 500 lines. The overall sum of line strengths has been calculated to be $127 \text{ cm}^{-2} \text{ atm}^{-1}$ at 296 K.

Preliminary results for the strengths of the ν_2 and ν_4 bands of $^{13}\text{CH}_4$ will be also presented.

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FC1.

(8:30)

AN IMPROVED METHOD FOR THE DIRECT COMPUTATION OF DIATOMIC
CENTRIFUGAL DISTORTION CONSTANTS

JOEL TELLINGHUISEN

A new algorithm for the numerical solution of inhomogeneous second-order differential equations is applied to the perturbation theory calculation of centrifugal distortion constants in diatomic molecules. The new scheme is similar to that of Hutson and Howard^{1, 2} but entails a combined inward and outward generation of the solution, analogous to that which is used in the Cooley³ routine for solving the analogous homogeneous equation. The matching at an intermediate point eliminates instabilities in the nonclassical regions and permits a straightforward extraction of the desired particular solution from the initial numerical solution, which contains a component of the homogeneous solution. Numerical tests suggest that this method is capable of greater precision and efficiency than existing methods.

A "computer movie" will be used to illustrate the method.

¹J. M. Hutson and B. J. Howard, *Mol. Phys.* 41, 1113 (1980).

²J. M. Hutson, *J. Phys. B: At. Mol. Phys.* 14, 851 (1981).

³J. W. Cooley, *Math. Comput.* 15, 363 (1961).

Address of Tellinghuisen: Department of Chemistry, Vanderbilt University, Nashville, Tennessee 37235.

FC2.

(8:47)

ANALYSIS OF THE D' + A' TRANSITION IN THE EMISSION SPECTRUM OF Cl₂

BAOCHUAN GUO, DILIP K. CHAKRABORTY, AND JOEL TELLINGHUISEN

The emission spectrum of Cl₂ in Ar is re-examined using Tesla discharge sources containing isotopically pure ³⁵Cl₂ and ³⁷Cl₂.¹ Earlier speculation that the dominant emission near 2580 Å is due to the D' 2_g(³P₂) → A' 2_u(³Π) transition is confirmed, with the following constants (in cm⁻¹) obtained for these states: ΔT_e = 40125.4, ω_e' = 253.17, ω_ex_e' = 1.14, ω_e'' = 257.27, ω_ex_e'' = 4.86. This same transition is also primarily responsible for the long-known² transient absorption spectrum of photoflashed Cl₂, which was previously interpreted in terms of absorption from the B 3_Π0⁺_u state. The emission spectrum contains weaker contributions from a second band system, tentatively assigned as B 1_g(³P₂) → A 1_u(³Π).

A rotational analysis of D' + A' is now in progress and will be reported.

¹J. Tellinghuisen and D. K. Chakraborty, *Chem. Phys. Lett.* (in press).

²A. G. Briggs and R. G. W. Norrish, *Proc. Roy. Soc. London* A276, 51 (1963).

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Current Address of Chakraborty: Department of Chemistry, University of Nevada at Reno, Reno, Nevada 89557.

TRANSITION STRENGTHS IN THE B - X SYSTEM OF I₂ FROM LINE ABSORPTION MEASUREMENTS

JOEL TELLINGHUISEN, DILIP K. CHAKRABORTY, AND MARCUS MENDENHALL

The intensity properties of the B $^3\Pi_0^+$ - X $^1\Sigma_g^+$ transition in I₂ have been studied extensively using absorption, fluorescence, stimulated emission, lifetime methods, and optical coherent transients. Although the electronic transition moment function $\mu_e(R)$ is now thought to be reasonably well known, there remain puzzling discrepancies among the many sets of results reported on this problem. In the present work we have attempted to resolve some of the inconsistencies by means of very high resolution absorption measurements of individual rotational lines, obtained using a single-frequency cw dye laser as source. Results will be reported for measurements in the range 5200-6700 Å.

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CONSTANTS OF THE 5S $^1\Sigma_g^+$ STATE OF Na₂ FROM TWO-PHOTON SPECTROSCOPY

G.-Y. YAN, T. P. DUFFEY, and A. L. SCHAWLOW

Fluorescence spectroscopy, following two-photon excitation of Rydberg levels in molecular sodium, has been performed. Several methods are introduced and used to identify those two-photon transitions and analyzed the spectra. Using these methods, the rotational quantum number, energy and electronics character of the upper level may be determined without any assumptions about the state to which the upper level belongs.

Twenty-nine two-photon transitions were observed. Most of them were associated with the $^1\Sigma_g^+$ (3S-5S) state and used to calculate new values of the Dunham coefficients for that state. These were in close agreement with values obtained in polarization labeling experiments.¹

¹A. J. Taylor, K. M. Jones, and A. L. Schawlow, J. Opt. Soc. Am. 73, 994 (1983).

Department of Physics, Stanford University, Stanford, CA 94305-4060.
Work supported by the National Science Foundation, Grant NSF PHY-86-04441.

FC5.

(9:38)

SPECTROSCOPIC STUDY OF THE $E^1\Sigma_g^+$ "SHELF" STATE IN ${}^7\text{Li}_2$

C. A. TOMCZYK, R. A. BERNHEIM, L. P. GOLD, and C. R. VIDAL

The $E^1\Sigma_g^+$ "shelf" state of the ${}^7\text{Li}_2$ molecule was investigated using a pulsed optical optical double resonance technique. The measurements cover the vibrational levels in the range $0 < v < 29$ including the shelf region around $13 < v < 15$. Molecular constants have been determined. Using an inverted perturbation approach an effective potential energy curve has been generated within the adiabatic approximation whose quantum mechanical energy eigenvalues reproduce the measured term values to within 0.113 cm^{-1} for the range $0 < v < 23$ and $0 < J < 47$.

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Address of Bernheim and Gold: Department of Chemistry, The Pennsylvania State University, 152 Davey Laboratory, University Park, PA 16802.
Address of Vidal: Max Planck-Institut für Extraterrestrische Physik, D-8046 Garching, Federal Republic of Germany.

FC6.

(9:55)

ZEEMAN EFFECT IN THE DOPPLER-FREE POLARIZATION SPECTROSCOPY OF THE $b^3\Pi_u$ STATE OF ${}^6\text{Li}_2$: FINE STRUCTURE CONSTANTS

W. H. JENG, XINGBIN XIE, L. P. GOLD, AND R. A. BERNHEIM

The Zeeman splitting of the Doppler-free polarization spectra of the singlet-triplet perturbed levels $A^1\Sigma_u^+$ ($v=2, J=33$); $b^3\Pi_u$ ($v=0, N=32, F1, e$) in ${}^6\text{Li}_2$ has been used to determine the fine structure constants for the triplet state. Measurements were made in magnetic fields up to 3 kG using a CW single mode dye laser. Orientation of the laser beam polarization with respect to the applied magnetic field gives different m_j level selectivity. A fit of the Zeeman splitting pattern vs magnetic field with a Hamiltonian containing vibronic, rotational, spin-orbit, spin-spin, spin-rotation, and Zeeman terms yields the interactions responsible for the fine structure.

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Address of Gold and Bernheim: Department of Chemistry, The Pennsylvania State University, 152 Davey Laboratory University Park, PA 16802.

FC7.

 ${}^6\text{Li}$ - ${}^7\text{Li}$ ISOTOPE EFFECTS IN THE $A^1\Sigma_u^+$ - $X^1\Sigma_g^+$ BAND SYSTEM OF Li_2

M. ELSHAKRE, R. A. BERNHEIM, C. M. FAUST, AND L. P. GOLD

The absorption spectrum of the A-X band system of ${}^6\text{Li}_2$ has been examined with a DA3.002 Fourier Transform Interferometer in the frequency range of $14,000-17,000 \text{ cm}^{-1}$. A resolution (0.01 cm^{-1}) spectrum was measured at two different temperatures in a heat pipe oven containing helium as a buffer gas. The spectrum was analyzed for vibrational coefficients and Franck-Condon factors. The molecular constants calculated were compared with those for ${}^7\text{Li}_2$.

Address of Elshakre, Bernheim, Faust, and Gold: Department of Chemistry, The Pennsylvania State University, 152 Davey Laboratory, University Park, PA 16802.

AD-A186 341

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COLUMBUS DEPT OF PHYSICS K N RAO 19 JUN 87

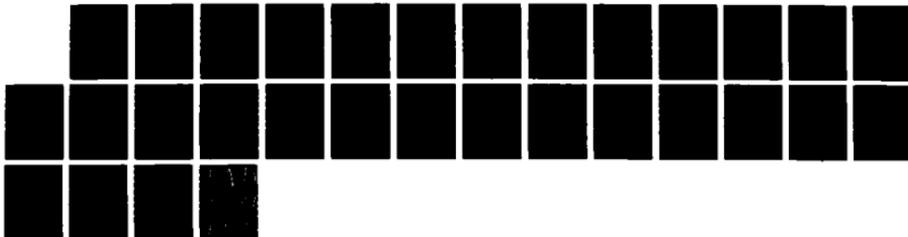
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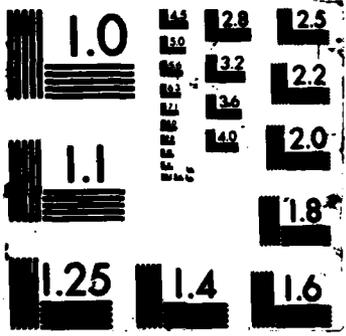
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FC8.

A SPECTROSCOPIC STUDY OF THE $1^1\Pi_g$ STATE OF $^7\text{Li}_2$

D. A. MILLER, R. A. BERNHEIM, AND L. P. GOLD

Previous studies of the excited electronic states of Li_2 in the visible and UV regions¹ has recently been extended into the infra-red. The $1^1\Pi_g$ state has been observed by pulsed optical optical double resonance of the metal vapor in a heat-pipe oven.

Following excitation to selected levels of the $A\ 1^1\Sigma_u^+$ state, the 2nd Stokes output of a hydrogen Raman shifter is directed into the oven. Transitions from $A\ 1^1\Sigma_u^+$ state levels to the $1^1\Pi_g$ state are detected by monitoring blue-green fluorescence as the Raman shifted light is scanned through the range, 1.1 μm -1.3 μm . The observations include 33 vibrational levels excited from $v=0$ in the A state. Molecular constants and a potential curve for the $1^1\Pi_g$ will be reported. Together with the recent FT-IR work of B. Barakat et al.², this study completes the observation of all singlet states arising from the $\text{Li}(2s) + \text{Li}(2p)$ dissociation limit.

¹R. A. Bernheim, L. P. Gold, and C. A. Tomczyk, in Comparison of Ab Initio Quantum Chemistry with Experiment for Small Molecules, Rodney J. Bartlett, ed. (D. Reidel Publ., Boston, 1985) and references therein.

²B. Barakat et al., *J. Mol. Spec.* **116**, 271-285 (1986).

Address of Bernheim, Gold, and Miller: Department of Chemistry, The Pennsylvania State University, 152 Davey Laboratory, University Park, PA 16802.

FC9.

ACCURATE DISSOCIATION ENERGIES FOR THE $X^1\Sigma^+$ STATES OF KH AND CsH

Warren T. Zemke and William C. Stwalley

We have constructed a new hybrid potential energy curve for the X state of KH that includes scaled ab initio calculations at short range, RKR turning points in the potential well and proper long-range behavior. Then for the observed¹ quasibound state ($v'' = 23$, $J'' = 7$, width = $0.40\ \text{cm}^{-1}$), we calculated line widths for varying binding energies. From a comparison with the experimental line width, we determined an improved dissociation energy $D_e = 14772.7 \pm 0.5\ \text{cm}^{-1}$. This result is $4.3\ \text{cm}^{-1}$ lower and eight times more precise than the best previous result based on $A^1\Sigma^+ - X^1\Sigma^+$ fluorescence experiments.¹

A new hybrid potential was also constructed for the X state of CsH . From a comparison of the experimental line width² for the observed quasibound state ($v'' = 25$, $J'' = 11$, width = $0.6\ \text{cm}^{-1}$), we determined an improved dissociation energy $D_e = 14792.3 \pm 1.4\ \text{cm}^{-1}$. This result is $15.7\ \text{cm}^{-1}$ lower and three times more precise than (but outside the range of) the best previous result from $A^1\Sigma^+ - X^1\Sigma^+$ fluorescence studies.²

¹ K. Hussein, C. Effantin, J. D'Incan, J. Vergés and R. F. Barrow, *Chem. Phys. Lett.* **124**, 105 (1986).

² C. Crepin, J. Vergés and C. Amiot, *Chem. Phys. Lett.* **112**, 10 (1984).

Address of Zemke: Department of Chemistry, Wartburg College, Waverly, Iowa 50677.

Address of Stwalley: Iowa Laser Facility and Departments of Chemistry and Physics, University of Iowa, Iowa City, Iowa 52242-1294.

FC10.

(11:06)

LASER-INDUCED FLUORESCENCE FROM THE $B^2\Sigma^+$ AND $B'^2\Delta$ STATES OF THE SiCl RADICAL*JAY B. JEFFRIES AND RICHARD A. COPELAND

Laser-induced fluorescence (LIF) is observed following excitation of ground state SiCl molecules to either the $B^2\Sigma^+$ or the $B'^2\Delta$ excited electronic states. Pulsed frequency-doubled light from an excimer-pumped dye laser excites the radicals in the afterglow of a low-pressure microwave discharge in He with a trace of added SiCl_4 . The fluorescence from $v' = 0-3$ of the $B^2\Sigma^+$ state and $v' = 0-1$ of the $B'^2\Delta$ state is dispersed with 2 nm resolution and the relative vibrational band strengths are measured for $v'' \leq 10$ in $B^2\Sigma^+ - X^2\Pi$ emission and $v'' \leq 3$ in $B'^2\Delta - X^2\Pi$ emission.

From the temporal evolution of the LIF, the fluorescence lifetimes of the B and the B' state are found to be ≤ 25 ns and 1.7 ± 0.5 μs , respectively. This large difference in the time behavior of the LIF allows the overlapped excitation spectra to be clearly separated with different time gates. Preliminary analysis of the helium pressure dependence of the fluorescence from the $B'^2\Delta$ indicates a collisional removal rate of $\sim 6 \times 10^{-11}$ cm^3s^{-1} . The dispersed fluorescence from the $B'^2\Delta$, $v' = 0$ state reveals a significant relaxation pathway is electronic-to-electronic collisional energy transfer to $v' = 0-2$ in $B^2\Sigma^+$. The large magnitude of the collisional removal rate of the B' state by He is very surprising and further investigations are currently underway.

*Supported by Internal Research and Development funds of SRI International

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FC11.

(11:23)

THE SPECTRUM OF ZrS R. J. WINKEL, JR.

Diatomic zirconium sulfide is a molecule of astrophysical interest.¹

A laboratory sample of zirconium disulfide powder and solid zirconium was heated in a King furnace to a temperature of 2150°C in a helium environment at 50 Torr. The emission spectrum was measured using the Fourier transform spectrometer at the National Solar Observatory at Kitt Peak. The spectral region 600-1000 nm was observed.

Results will be discussed. A number of molecular bandhead features were identified and attributed to ZrS .

¹D. L. Lambert and R. E. S. Clegg, Mon. Not. R. Astr. Soc. 191, 367 (1980).

Address: Department of Physics, United States Military Academy, West Point, New York, 10997-1790.

FC12.

(11:35)

SUB-DOPPLER SPECTROSCOPY OF THE $A^6\Sigma^+ - X^6\Sigma^+$ TRANSITION OF MnSM. Douay, B. Pinchemel and C. Dufour

MnS was produced in a Broida-type oven by the oxidation of manganese vapor by carbonyl sulfide.

The 0-1 band of the $A^6\Sigma^+ - X^6\Sigma^+$ electronic transition was observed by intermodulated fluorescence spectroscopy (about 90 MHz resolution) in the range 18300-18375 cm^{-1} . The hyperfine structure, caused by the Mn nucleus ($I=5/2$), exhibits a regular Lande pattern except for the F_3 and F_4 electronic spin-components. The hyperfine matrix elements of the type $\Delta J=1$ caused an internal hyperfine perturbation of the F_3 and F_4 electronic spin-components in both the A and X states. The Fermi contact term in the ground state is smaller in MnS than in MnO, indicating that the bonding in MnS is more covalent than in MnO.

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FC13.

(11:52)

ROTATIONAL ANALYSIS OF THE $A^1\Sigma^+ - X^1\Sigma^+$ TRANSITION OF SrSF.S. Pianalto, C.R. Brazier, L.C. O'Brien, and P.F. Bernath

The laser induced fluorescence spectrum of strontium monosulfide (SrS) was recorded. SrS was produced by the reaction of strontium vapor and carbon disulfide (CS_2) in a Broida oven. The 0-0, 0-1, 1-1, 3-0, 4-1, 5-1, and 5-2 vibrational bands of the previously unobserved $A^1\Sigma^+ - X^1\Sigma^+$ electronic system were measured and analyzed. Spectra and molecular constants will be presented.

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FC14.

(12:04)

ANOMALOUS POPULATION DISTRIBUTION IN THE $2c^3\Pi_u$ STATE OF MOLECULAR HYDROGENG. O. Brink, K. H. Kim, and A. K. Banerjee

We have observed about 700 lines of the absorption spectrum of molecular hydrogen arising from transitions between the $2c^3\Pi_u$ state and the $n=3 \Sigma\Pi_V$ complex using the technique of dye laser intracavity absorption. Because of the nature of the energy levels one component of the λ doublet of each rotational level of the $2c$ state predissociates with a lifetime of the order of 2×10^{-9} sec. while the non-predissociative component has a lifetime of about 8×10^{-5} sec. for radiative decay. This would suggest that the density of molecules in the predissociative states should be at least a factor of 10^{-5} smaller than that of the non-predissociative state.

Our data shows that in an rf produced hydrogen plasma the intensities of the two kinds of transitions are comparable. The linearity of our ICA system has been demonstrated by measuring the quenching rate of the $2c$, $v=2$, $N=1$ state by Ne, and obtaining the same result given by Tischer and Phelps¹. Our data suggests that there is a mechanism operating in the plasma which preferentially populates the predissociative states, and some suggestions as to its nature will be presented.

¹H. Tischer and A. V. Phelps, Chem. Phys. Lett. 117, 550 (1985)

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Address of Kim: Department of Physics and Engineering,
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THE OHIO STATE UNIVERSITY, COLUMBUS, OHIO

1987 SYMPOSIUM ON MOLECULAR SPECTROSCOPY

JUNE 15-19, 1987

This list consists mostly of participants who have made reservations in the dormitory. Their room numbers are available at the Drackett Tower Dormitory located at 161 Curl Drive(292-8611).

Asterisks are used for the participants residing off campus. Their location can be obtained at the registration desk in the Physics Building. Lists of other participants will be made available during the symposium as they register.

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1987 SYMPOSIUM ON MOLECULAR SPECTROSCOPY
THE OHIO STATE UNIVERSITY, COLUMBUS, OHIO

MONDAY, JUNE 15, 1987

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1987 SYMPOSIUM ON MOLECULAR SPECTROSCOPY
THE OHIO STATE UNIVERSITY, COLUMBUS, OHIO

TUESDAY, JUNE 16, 1987

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