AL-TR-90-025 AD:

AD-A225 503

Final Report
for the period
17 February 1987 to
16 February 1990

Laser and Fourier Transform Spectroscopy of Novel Propellant Molecules

July 1990

Author:
P. F. Bernath

Approved for Public Release

Astronautics Laboratory (AFSC)
Air Force Space Technology Center
Space Systems Division
Air Force Systems Command
Edwards AFB CA 93523-5000

NOTICE TO ACCOMPANY THE DISSEMINATION OF EXPORT-CONTROLLED TECHNICAL DATA

1. Export of information contained herein, which includes, in some circumstances, release to foreign nationals within the United States, without first obtaining approval or license from the Department of State for items controlled by the International Traffic in Arms Regulations (ITAR), or the Department of Commerce for items controlled by the Export Administration Regulations (EAR), may constitute a violation of law.

2. Under 22 U.S.C. 2778 the penalty for unlawful export of items or information controlled under the ITAR is up to 2 years imprisonment, or a fine of $100,000, or both. Under 50 U.S.C., Appendix 2410, the penalty for unlawful export of items or information controlled under the EAR is a fine up of up to $1,000,000, or five times the value of the exports, whichever is greater; or for an individual, imprisonment of up to 10 years, or a fine of up to $250,000, or both.

3. In accordance with your certification that establishes you as a "qualified U.S. contractor," unauthorized dissemination of this information is prohibited and may result in disqualification as a qualified U.S. contractor, and may be considered in determining your eligibility for future contracts with the Department of Defense.

4. The U.S. Government assumes no liability for direct patent infringement, or contributory patent infringement or misuse of technical data.

5. The U.S. Government does not warrant the adequacy, accuracy, currency, or completeness of the technical data.

6. The U.S. Government assumes no liability for loss, damage, or injury resulting from manufacture or use for any purpose of any product, article, system, or material involving reliance upon any or all technical data furnished in response to the request for technical data.

7. If the technical data furnished by the Government will be used for commercial manufacturing or other profit potential, a license for such use may be necessary. Any payments made in support of the request for data do not include or involve any license rights.

8. A copy of this notice shall be provided with any partial or complete reproduction of these data that are provided to qualified U.S. contractors.

NOTICE

When U. S. Government drawings, specifications, or other data are used for any purpose other than a definitely related Government procurement operation, the fact that the Government may have formulated, furnished, or in any way supplied the said drawings, specifications, or other data, is not to be regarded by implication or otherwise, or in any way licensing the holder or any other person or corporation, or conveying any rights or permission to manufacture, use or sell any patented invention that may be related thereto.

FOREWORD

This final report was submitted by University of Arizona, on completion of Contract F04611-87-K-0020 with the Astronautics Laboratory (AFSC), Edwards AFB CA. AL Project Manager was Lt Roeland Van Opijnen.

This report has been reviewed and is approved for release and distribution in accordance with the distribution statement on the cover and on the DD Form 1473.

Roeland Van Opijnen

ROELAND VAN OPIJNEN, LT, USAF
Project Manager

Stephen L. Rodgers

STEPHEN L. RODGERS
Chief, Advanced Research in Energy Storage Office

FOR THE DIRECTOR

Robert C Corley

ROBERT C. CORLEY
Director, Astronautical Sciences Division

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE

REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for Public Release; Distribution is Unlimited
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S) AL-TR-90-025
6a. NAME OF PERFORMING ORGANIZATION University of Arizona 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION Astronautics Laboratory (AFSC)
6c. ADDRESS (City, State, and ZIP Code) Department of Chemistry Tuscon AZ 85721	7b. ADDRESS (City, State, and ZIP Code) AL/LSX Edwards AFB CA 93523-5000
8a. NAME OF FUNDING/SPONSORING ORGANIZATION 8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER F04611-87-K-0020
8c. ADDRESS (City, State, and ZIP Code)	10. SOURCE OF FUNDING NUMBERS

PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT ACCESSION NO.
62302F	5730	00	9G

11. TITLE (Include Security Classification)

Laser and Fourier Transform Spectroscopy of Novel Propellant Molecules (U)

12. PERSONAL AUTHOR(S)

Bernath, Peter F.

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final	FROM 870217 TO 900216	9007	25

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	
07	03		
07	05		

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

A wide variety of energetic molecules have been studied by the techniques of Fourier transform spectroscopy and visible laser spectroscopy. Molecules observed include N_3, SiC, C_2, C_3, C_5, He_2, XeH, BH, BD, CCN, $CaBH_4$ and $SrBH_4$. These molecules were detected by absorption or emission measurements in the infrared, visible and ultraviolet regions of the spectrum.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS	UNCLASSIFIED
22a. NAME OF RESPONSIBLE INDIVIDUAL Lt Roeland van Opijnen	22b. TELEPHONE (Include Area Code) (805) 275-5725 22c. OFFICE SYMBOL AL/LSX

DD Form 1473, JUN 86 *Previous editions are obsolete.*

SECURITY CLASSIFICATION OF THIS PAGE

UNCLASSIFIED

TABLE OF CONTENTS

		PAGE
	Summary	i
A.	Introduction	1
B.	Trinitrogen, N_3	1
C.	Silicon carbide, SiC	2
D.	Dicarbon, C_2	3
E.	Tricarbon and Pentacarbon, C_3 and C_5	4
F.	Rydberg Molecules, He_2 and XeH	6
G.	Boron Hydrides and Deuteride, BH and BD	8
H.	Boron Carbide, BC	8
I.	Dicarbon nitride, CCN	10
J.	Metal Monoborohydrides, $CaBH_4$ and $SrBH_4$	10
K.	Conclusions and Future Directions	11
L.	Publications (supported by F04611-87-K-0020)	11

Summary

A wide variety of energetic molecules have been studied by the techniques of Fourier transform spectroscopy and visible laser spectroscopy. Molecules observed include N_3, SiC, C_2, C_3, C_5, He_2, XeH, BH, BD, CCN, $CaBH_4$ and $SrBH_4$. These molecules were detected by absorption or emission measurements in the infrared, visible and ultraviolet regions of the spectrum. The antisymmetric stretching vibration of N_3 was detected in absorption near 1645 cm^{-1}. New Fourier transform electronic emission spectra of SiC, C_2 and C_3 were found in the infrared. Infrared electronic emission spectra were also recorded for the Rydberg molecules He_2 and XeH. Infrared vibration-rotation absorption spectra of C_3 and C_5 were discovered in a carbon star. Visible emission spectra of BH, BD and CCN were recorded with the Kitt Peak Fourier transform interferometer. For CCN, ultra-cold emission from a free radical jet expansion source was analyzed. $CaBH_4$ and $SrBH_4$ were made by the reaction of Ca and Sr vapors with diborane, B_2H_6, and detected by laser-induced fluorescence.

A. INTRODUCTION

The goal of our work is the exploration of the spectroscopy of a wide variety of energetic molecules. Many of these molecules store considerable energy by virtue of large positive heats of formation. To make suitable propellants these species must be stabilized so that they can be stored and released on demand. However, the first step is the discovery and spectroscopic characterization of these unusual new molecules.

The principal tool in our quest for new molecules is the high-resolution Fourier transform spectrometer. We have made extensive use of the exceptional instrument associated with the McMath Solar Telescope operated by the National Solar Observatory at Kitt Peak.

B. Trinitrogen, N_3

The antisymmetric stretching vibration, ν_3, of N_3 was measured in absorption[1] near 1645 cm^{-1}. No previous high-resolution infrared measurements for this very energetic free radial are available. The spectrum of N_3 was recorded in absorption with the unique fast flow White cell of C. Howard of NOAA in Boulder, Colorado, with a BOMEM Fourier transform spectrometer. The N_3 radical was made by the reaction of Cl radicals and HN_3. The Cl atoms were made by discharging 0.02% Cl_2 in He while HN_3 was produced by the reaction of NaN_3 with molten stearic acid. The total pressure in the White cell was about 200 mtorr.

Molecular constants for the 000 and 001 vibrational levels of the ground $\tilde{X}^2\Pi_g$ state were determined (Table I). The vibrational frequency of 1645 cm^{-1} for the antisymmetric stretch of N_3 was lower than expected by analogy with similar molecules. This gas-phase value agrees with the recent Ar matrix value of 1658 cm^{-1} found by Tian, Facelli and Michl [*J. Phys. Chem.* **92**, 4073 (1988)].

TABLE I

Molecular Constants for the ν_3 Band of N_3 (in cm^{-1})

	Constant	000	001
	ν_3	--	1644.67832(4)[a]
	A	-71.2729(18)	-70.8909(18)
10^6	A_D	-8.84(95)	2.99(94)
	B	0.4314495(13)	0.4270645(13)
10^7	D	1.886(10)	1.885(10)
10^3	p	1.357(73)	1.561(72)
10^4	q	-0.613(28)	-1.392(27)

[a] Numbers in parentheses represent one standard deviation error estimates in the last significant figure.

C. Silicon Carbide, SiC

SiC is a very elusive molecule. Although C_2 and Si_2 are well-known molecules, SiC escaped detection until our discovery of the

infrared electronic transition[2] $d^1\Sigma^+ - b^1\Pi$ near 6100 cm^{-1} (Figure 1). An energy level diagram is provided in Figure 2. In our experiment, SiC was sputtered from a pressed composite wall hollow cathode made from a 3:1 mixture of Cu and SiC powders. The hollow cathode was operated at 200 mA with a slow flow of 1.5 Torr of neon gas. Sixty-nine scans were co-added in 8.3 hours of integration with a spectrometer resolution of 0.02 cm^{-1}.

In this work the collaboration of A. D. McLean was critical because without his *ab initio* calculations we could not assign our spectrum. In fact, with our experimental r_o value for the $b^1\Pi$ state, he was able to calibrate his calculations and predict an r_o value for the ground $X^3\Pi$ state. This accurate prediction helped in the detection of the microwave spectrum of SiC in space and in the laboratory by Gottlieb, Thaddeus and co-workers [*Astrophys. J.* **341**, L25 (1989)]. Their microwave data, in turn, have now allowed us to assign another infrared electronic transition[3], $A^3\Sigma^- - X^3\Pi$, near 4600 cm^{-1} (Figure 2).

D. Dicarbon, C_2

In the course of our discovery of the SiC molecule, A. D. McLean pointed out to us that the $B'^1\Sigma^+$ state of C_2 was unknown (Figure 3). This state corresponds to the newly discovered $d^1\Sigma^+$ state (Figure 2) of the isovalent SiC molecule. This was quite surprising since C_2 occurs in a wide variety of sources such as flames and C_2 has been studied for many years. Examination of two previously recorded spectra of hydrocarbon discharges disclosed two new infrared electronic

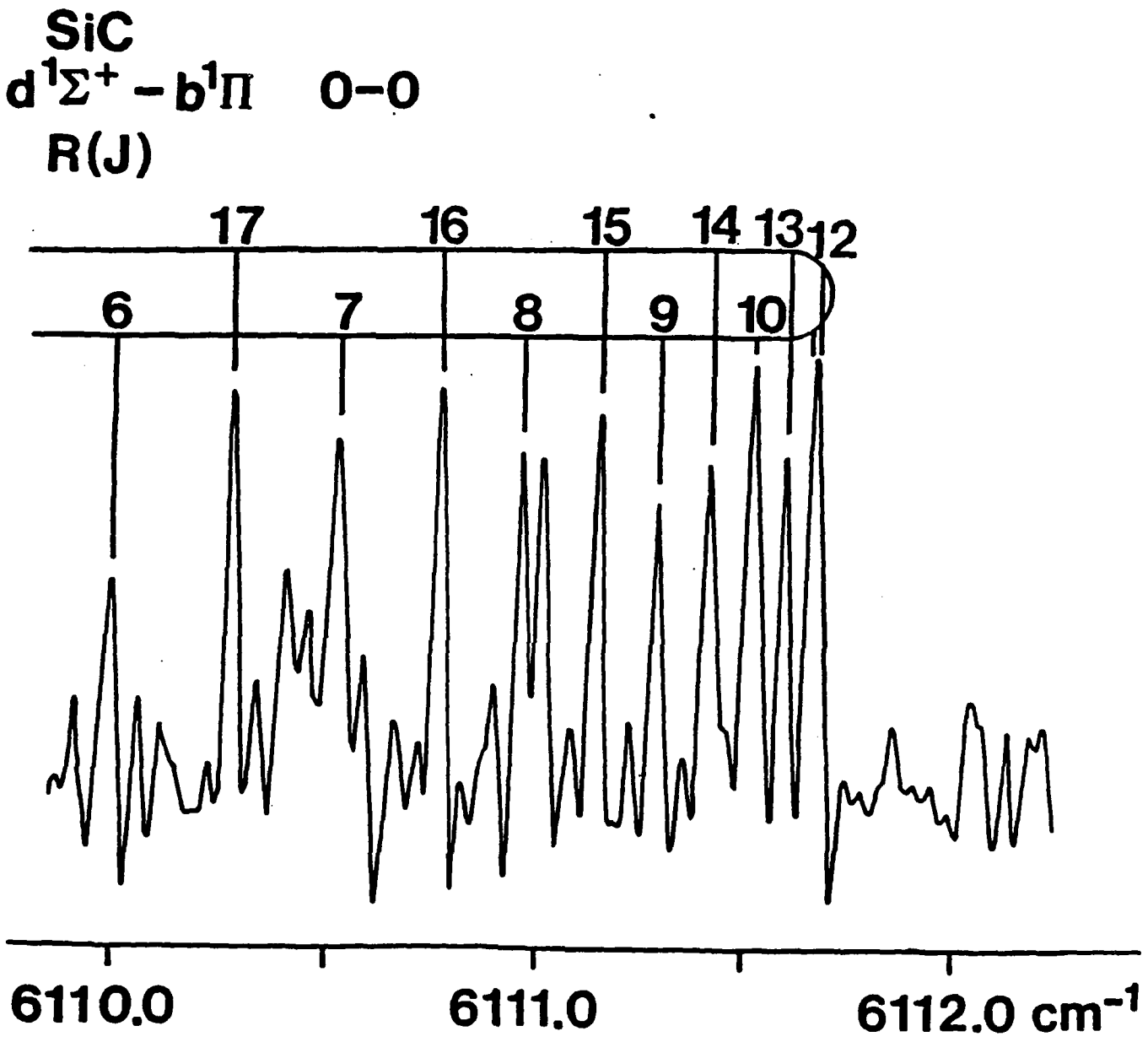

FIGURE 1

A portion of the 0-0 band of the $d^1\Sigma^+ - b^1\Pi$ spectrum of SiC near the R band head.

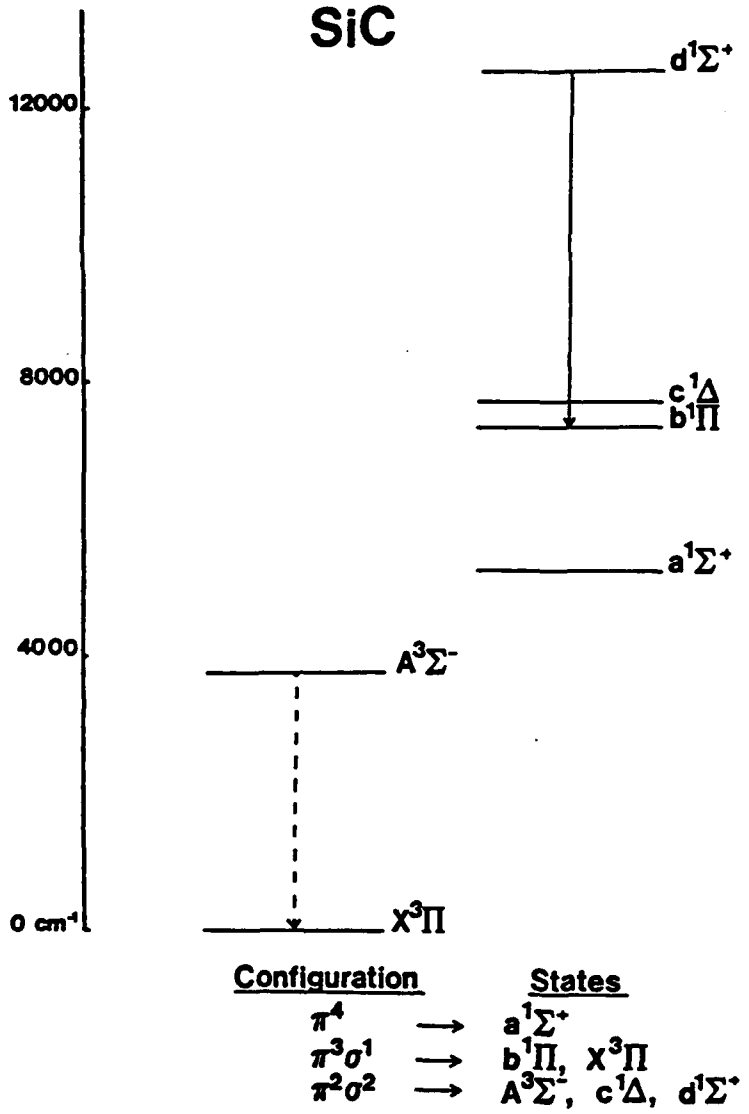

FIGURE 2

The low-lying states of SiC, as predicted by the *ab initio* calculations of Bernath *et al.* (Publication #2). The $d^1\Sigma^+ - b^1\Pi$ and $A^3\Sigma^- - X^3\Pi$ electronic transitions have been analyzed.

tra of hydrocarbon discharges disclosed two new infrared electronic transitions[4] of C_2: $B'^1\Sigma_g^+ - A^1\Pi_u$ and $B^1\Delta_g - A^1\Pi_u$ (Figure 3).

These spectra were excited by an electrodeless microwave discharge of hydrocarbons in a quartz tube. In one run a mixture of 2.75 Torr of He, 0.030 Torr of CH_4 and 0.040 Torr of white phosphorous vapor flowed through the discharge tube. The phosphorous is, presumably, not required. The emission was detected with InSb detectors and a silicon filter in the 1800-9000 cm^{-1} region. Ten interferometer scans were co-added in 70 minutes of integration with a resolution of 0.02 cm^{-1}.

The $B^1\Delta_g$ and $B'^1\Sigma_g^+$ states were the two missing low-lying bound electronic states of C_2. These two states do not connect with the ground $X^1\Sigma_g^+$ state by one photon electric dipole selection rules. The infrared electronic transitions $B^1\Delta_g - A^1\Pi_u$ and $B'^1\Sigma_g^+ - A^1\Pi_u$ are, however, quite strong (Figure 4). These new transitions should be observable in comets, stellar atmospheres, flames and in the combustion of propellants.

In order to connect our new states to the ground $X^1\Sigma_g^+$ state, we also reanalyzed the Phillips system[5], $A^1\Pi_u - X^1\Sigma_g^+$. Two new vibrational levels (v" = 5 and 6) of the $X^1\Sigma_g^+$ state were found, as well as a much improved set of molecular constants.

E. Tricarbon and Pentacarbon, C_3 and C_5

The antisymmetric stretching mode of C_3 near 2040 cm^{-1} is well-known from matrix isolation spectroscopy but was only recently ob-

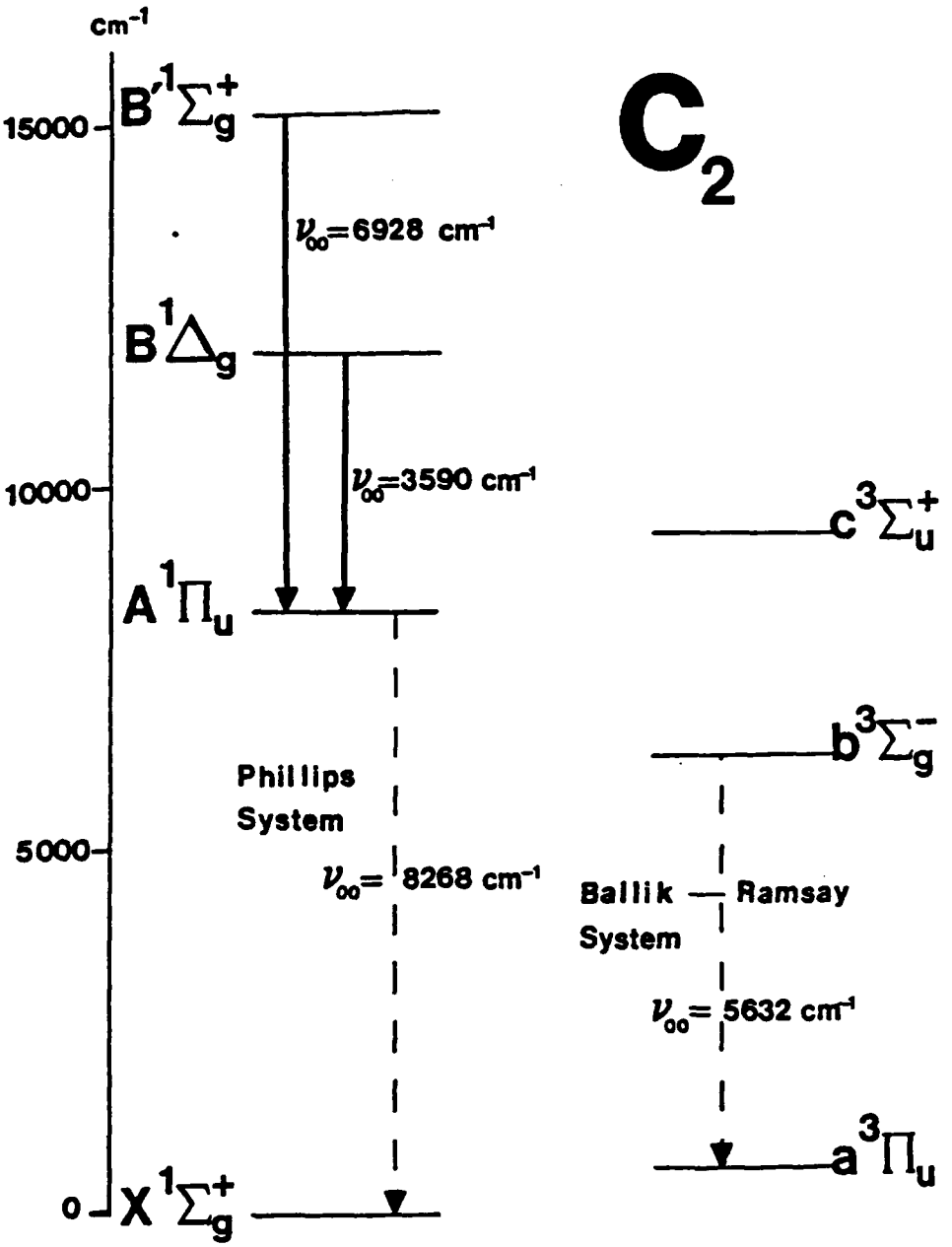

FIGURE 3

An energy level diagram of the low-lying states of C_2. The $B'^1\Sigma_g^+$ - $A^1\Pi_u$ and $B^1\Delta_g$ - $A^1\Pi_u$ infrared electronic transitions are described in this report.

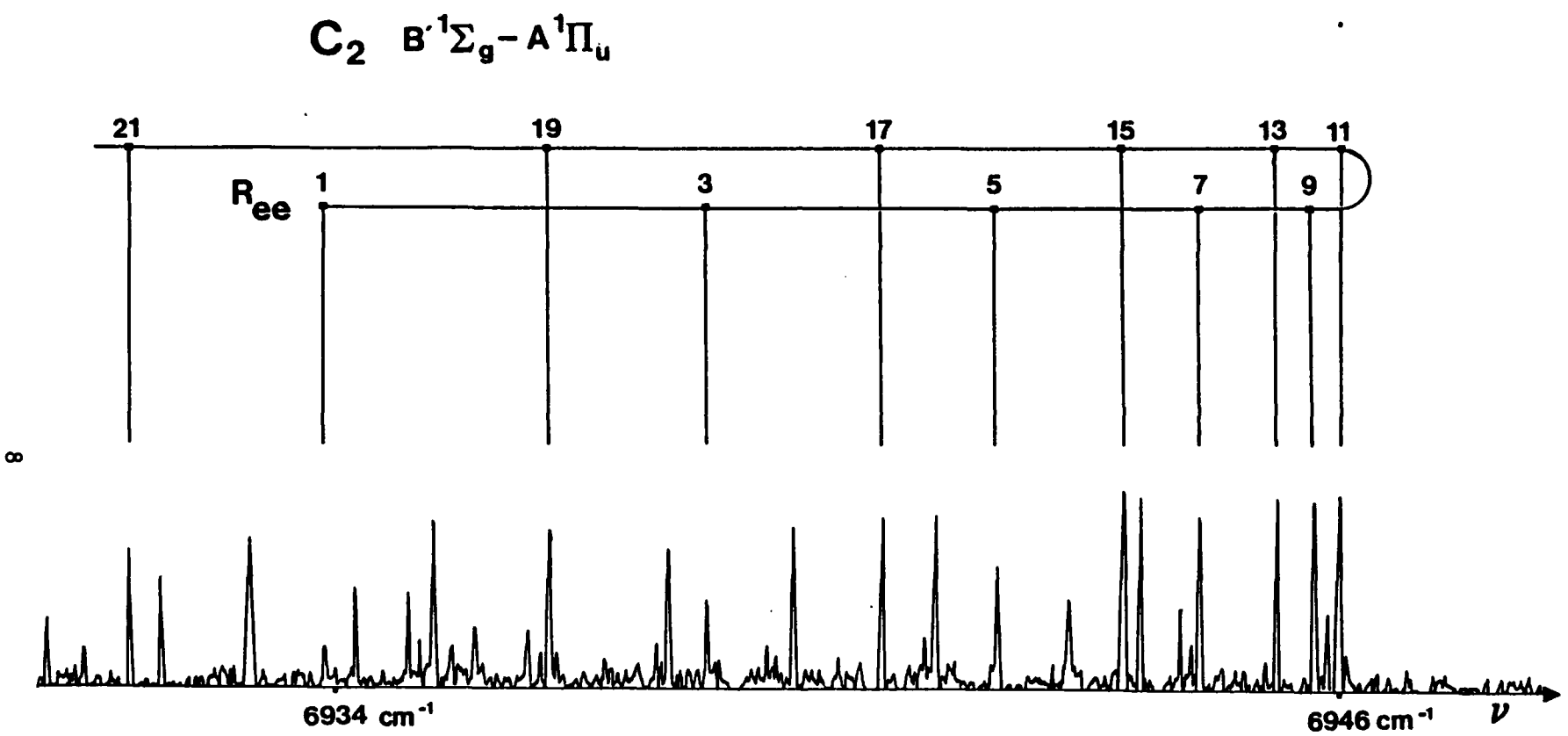

FIGURE 4

A portion of the 0-0 band of the $B'^1\Sigma_g^+ - A^1\Pi_u$ transition of C_2 near the R head. The corresponding R head for SiC is displayed in Figure 1.

served in the gas phase. We discovered[6] the ν_3 mode of C_3 in the infrared spectrum of a carbon star's atmosphere (Figure 5). Our spectroscopic constants for C_3 are provided in Table II. Hirota and coworkers [Matsumura, Kanamori, Kawaguchi and Hirota, *J. Chem. Phys.* **89**, 3491 (1988)] simultaneously found the laboratory spectrum of this mode of C_3.

The C_3 molecule was found to have a temperature of about 40K and was very abundant in this carbon star. Inspired by the C_3 results, we searched for and found the C_5 molecule in the same source. The ν_3 mode of C_5 was detected[7] near 2169 cm^{-1}, close to the argon matrix value of 2164 cm^{-1} [Vala, Chandrasekhar, Szczepanski, Van Zee and Weltner, *J. Chem. Phys.* **90**, 545 (1989)].

In collaboration with T. Amano and H. Sasada of the National Research Council of Canada, we have discovered the $\tilde{b}^3\Pi_g - \tilde{a}^3\Pi_u$ electronic transition of C_3 (Figure 6). This infrared electronic transition occurs near 6480 cm^{-1}. Although a long-lived, matrix-induced $\tilde{a}^3\Pi_u - \tilde{X}^1\Pi_g$ emission of C_3 is known near 17000 cm^{-1}, this work is the first gas-phase characterization of triplet states of C_3. The $\tilde{a}^3\Pi_u$ state of C_3 is a metastable energy reservoir. This triplet C_3 emission occurred in the same spectrum which contained the C_2 infrared emission.

Pure carbon molecules such as C_3, C_5 (and C_{60}) are in vogue as research topics. These molecules may be involved in many astrophysical processes, as well as in soot production in flames. Pure carbon molecules are also attractive as advanced propellants, if they can be stabilized.

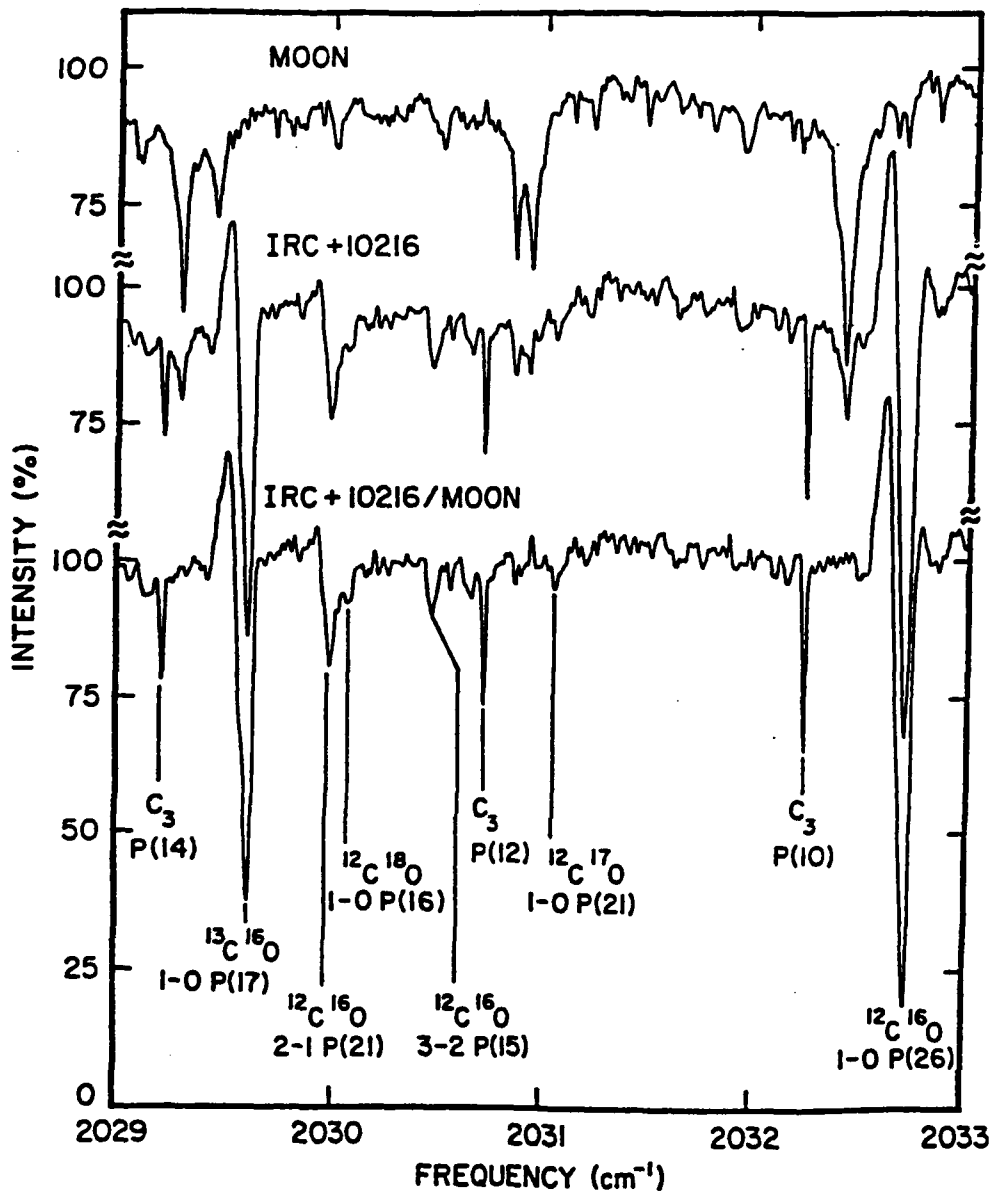

FIGURE 5

A short spectrum of the moon, the carbon star IRC+10216 and the ratio, IRC+10216/moon. The C_3 lines occur in absorption in the dusty envelope of this star. Note that the frequency scale has not been corrected for the earth's motion relative to the star.

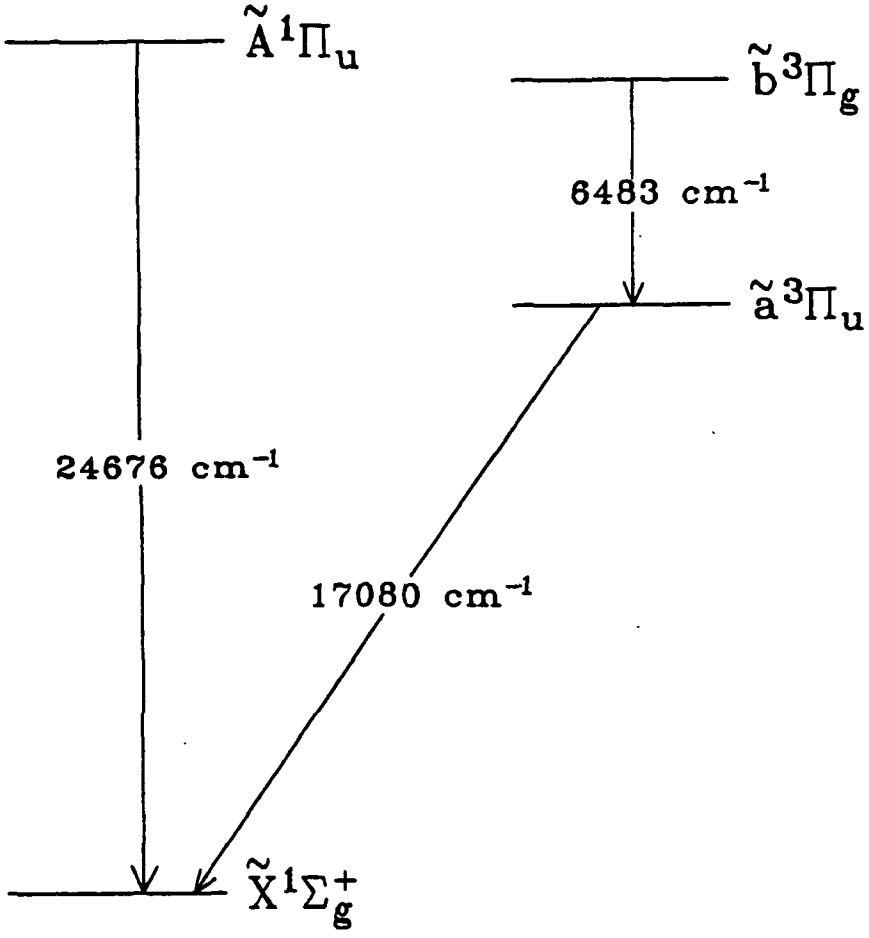

FIGURE 6

Energy level diagram of the low-lying states of C_3. The discovery of the $\tilde{b}^3\Pi_g$ - $\tilde{a}^3\Pi_u$ infrared transition is reported here.

TABLE II

Spectroscopic Constants for the ν_3 Vibrational Mode of C_3

Constant (cm^{-1})	Value
ν_3	2040.02113(62)[a]
$B_{0,0,0}$	0.430557(37)
$D_{0,0,0}$	$1.415(79)\times10^{-6}$
$B_{0,0,1}$	0.435654(39)
$D_{0,0,1}$	$3.937(88)\times10^{-6}$

[a] One standard deviation uncertainty in parentheses.

F. Rydberg Molecules, He_2 and XeH

He_2 and XeH are "Rydberg molecules" which have well-bound ionic He_2^+ and XeH^+ cores and weakly held outer electrons in Rydberg orbitals. By virtue of their electronic excitation, Rydberg molecules have a very high energy content.

The Fourier transform spectrometer of the National Solar Observatory at Kitt Peak was used to record infrared electronic emission spectra of XeH and He_2. For He_2, 0-0 and 1-1 bands of the $b^3\Pi_g - a^3\Sigma_u^+$ transition was observed near 4700 cm^{-1} at 0.01 cm^{-1} resolution.[8] The spectrum of He_2 was excited in a Ni hollow cathode operated at 280mA.

A flow of He gas at 4 torr pressure was maintained through the cathode. The precision of our measurements was ± 0.001 cm^{-1}.

Our measurements on He_2 fully resolve the triplet splittings of the $b^3\Pi_g - a^3\Sigma_u^+$ transition. These high-resolution observations provide a very precise set of molecular constants for He_2, including Λ-doubling constants for the $b^3\Pi_g$ state. Interpretation of the fine structure and Λ-doubling constants provide some insight into the electronic structure. For example, the $b^3\Pi_g$ state is in accidental pure precession with the nearby $c^3\Sigma_g^+$ state. The observed line positions, spectroscopic constants and other details are available in our paper published in *Molecular Physics*.[8]

The XeH Rydberg molecule was observed with the same techniques used for He_2. Instead of He, a slow, continuous flow of 2.2 torr of H_2 and 100 mtorr of Xe was maintained through the Ni hollow cathode tube. In our discharge an excess of hydrogen makes H_3^+, which then protonates Xe to make XeH^+. Recombination of XeH^+ with an electron gives rise to infrared electronic emission of XeH. The resolution of the Fourier transform spectrometer was 0.02 cm^{-1}.

The 0-0 vibrational bands of two new infrared electronic transitions were observed: The $D^2\Sigma^+ - C^2\Pi$ transition near 4420 cm^{-1} and the $C^2\Pi - B^2\Sigma^+$ transition near 3250 cm^{-1} (Figure 7). A rotational analysis provided spectroscopic constants[9] for the states connected by these transitions.

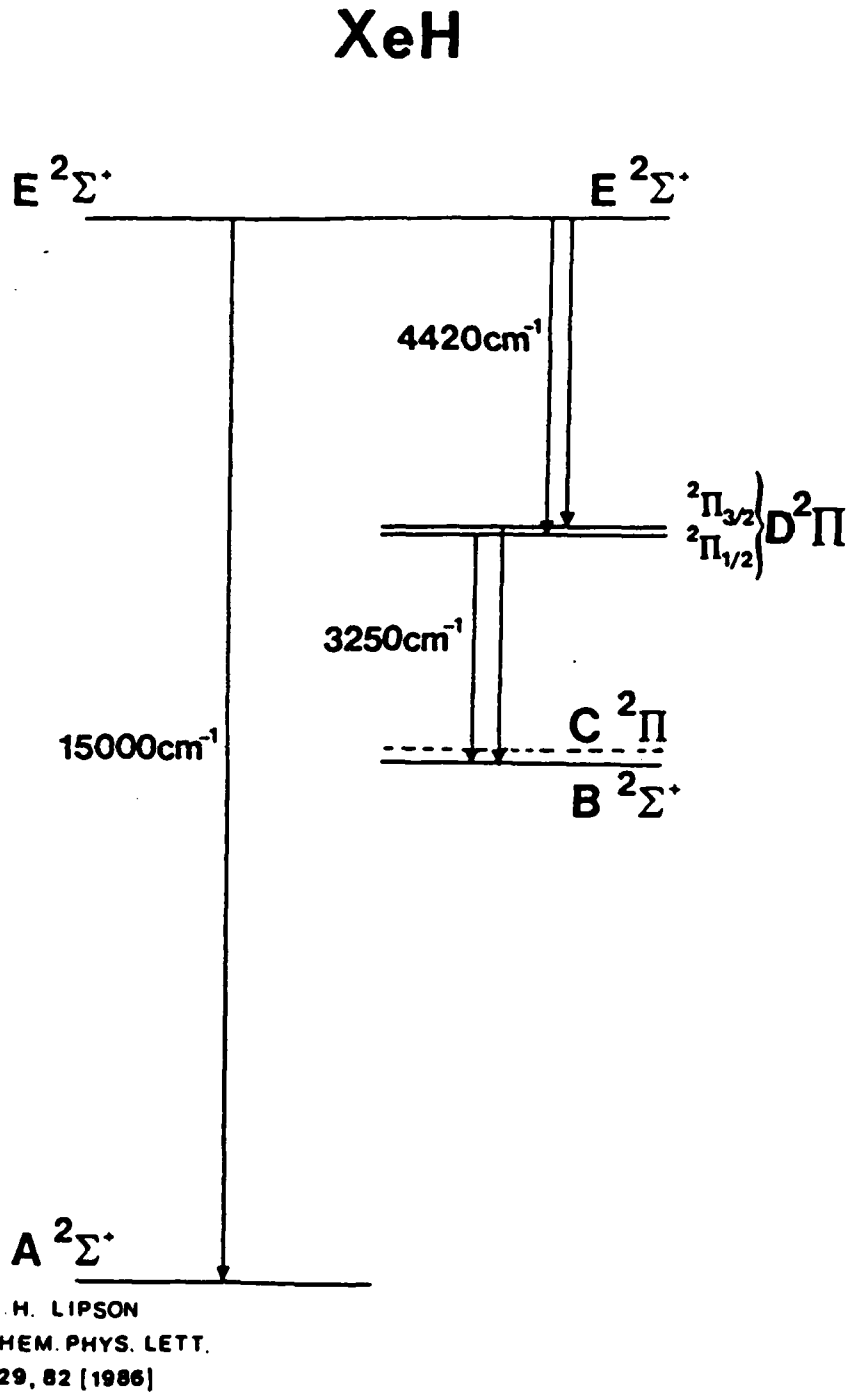

FIGURE 7

The low-lying states of the Rydberg molecule XeH. We have analyzed the $E^2\Sigma^+ - D^2\Pi$ and $D^2\Pi - B^2\Sigma^+$ infrared electronic transitions.

G. Boron Hydride and Deuteride, BH and BD

Boron derivatives, particularly borohydrides, are often suggested as advanced propellants. We discovered the vibration-rotation spectrum[10] of BH in a microwave discharge of diborane, B_2H_6. Although several electronic transitions of BH are well-known, the high-resolution infrared spectrum had not been previously detected.

The vibration-rotation emission spectrum of the BH $X^1\Sigma^+$ state was observed with the McMath Fourier transform spectrometer at Kitt Peak.[10] The 1-0, 2-1 and 3-2 bands were observed in a microwave discharge of 1 torr of He with 0.016 torr of B_2H_6. Spectroscopic constants of the individual vibrational levels and equilibrium molecular constants were determined. An RKR potential curve was calculated from the equilibrium constants.[10]

In the course of our work with BC (see below), we accidentally observed the $A^1\Pi$ - $X^1\Sigma^+$ transition of BH. Addition of a small amount of D_2 then provided the corresponding electronic transition of BD (Figure 8). Our reanalysis[11] resulted in much improved spectroscopic constants for BH and BD.

H. Boron Carbide, BC

Light elements with very stable oxides such as B and C are excellent propellants so we explored the simple binary BC system. Our production of BC was similar to our work with SiC. A composite wall (B_4C/Cu) hollow cathode discharge served as a light source for the Kitt Peak Fourier transform spectrometer. This composite wall

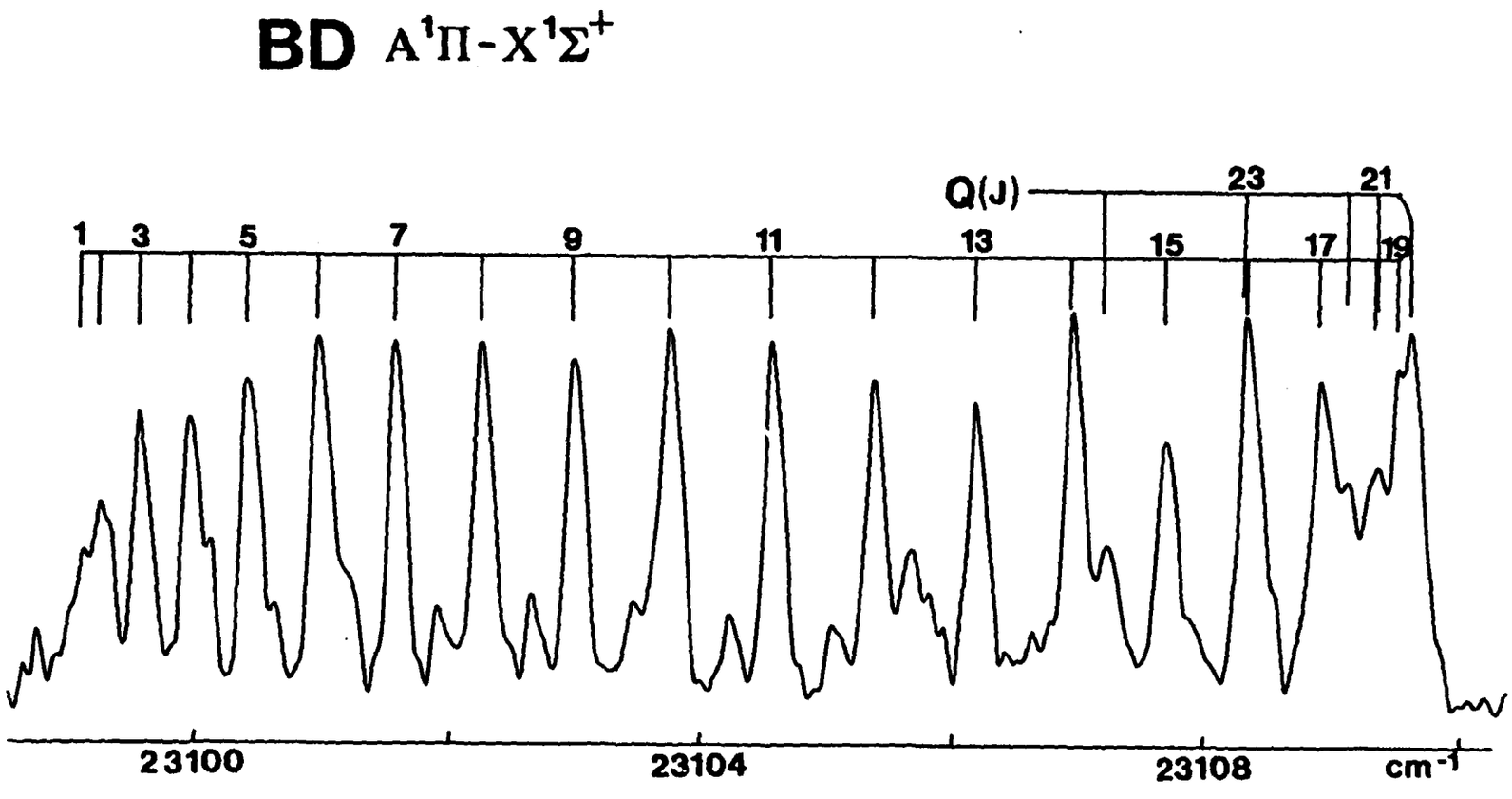

FIGURE 8

A short section of the Q branch of the 0-0 band of the $A^1\Pi$ - $X^1\Sigma^+$ transition of BD.

hollow cathode was very similar to the SiC/Cu cathode used for the production of SiC.

A current of 400 mA was maintained through a discharge in 1.2 Torr of flowing argon gas. Two cooled GaAs photomultiplier tubes (RCA 31034) were used as detectors. The spectra were integrated for about two hours with a resolution of about 0.02 cm^{-1}.

In the initial spectra, the $B^4\Sigma^- - X^4\Sigma^-$ transition of BC was very weak and the first lines were not detected. Some evidence of spin-splitting was found in the lines. We recently recorded much improved spectra containing the 0-0, 1-1, 2-2 and 3-3 bands of the B-X transition. These spectra allow an unambiguous rotational assignment and show evidence of the spin-splitting between the $^4\Sigma^-_{3/2}$ and $^4\Sigma^-_{1/2}$ components (Figure 9). The preliminary molecular constants [11] are provided in Table III.

TABLE III

Spectroscopic Constants for the 0-0 Band of the $B^4\Sigma^- - X^4\Sigma^-$ transition of BC (in cm^{-1}).

Constant	$B^4\Sigma^-$	$X^4\Sigma^-$
T_0	17904.8567(14)	--
B_0	1.369356(51)	1.311849(52)
$D_0 \times 10^5$	7.166(46)	7.492(45)
λ_0	-0.0462(33)	0.0275(32)

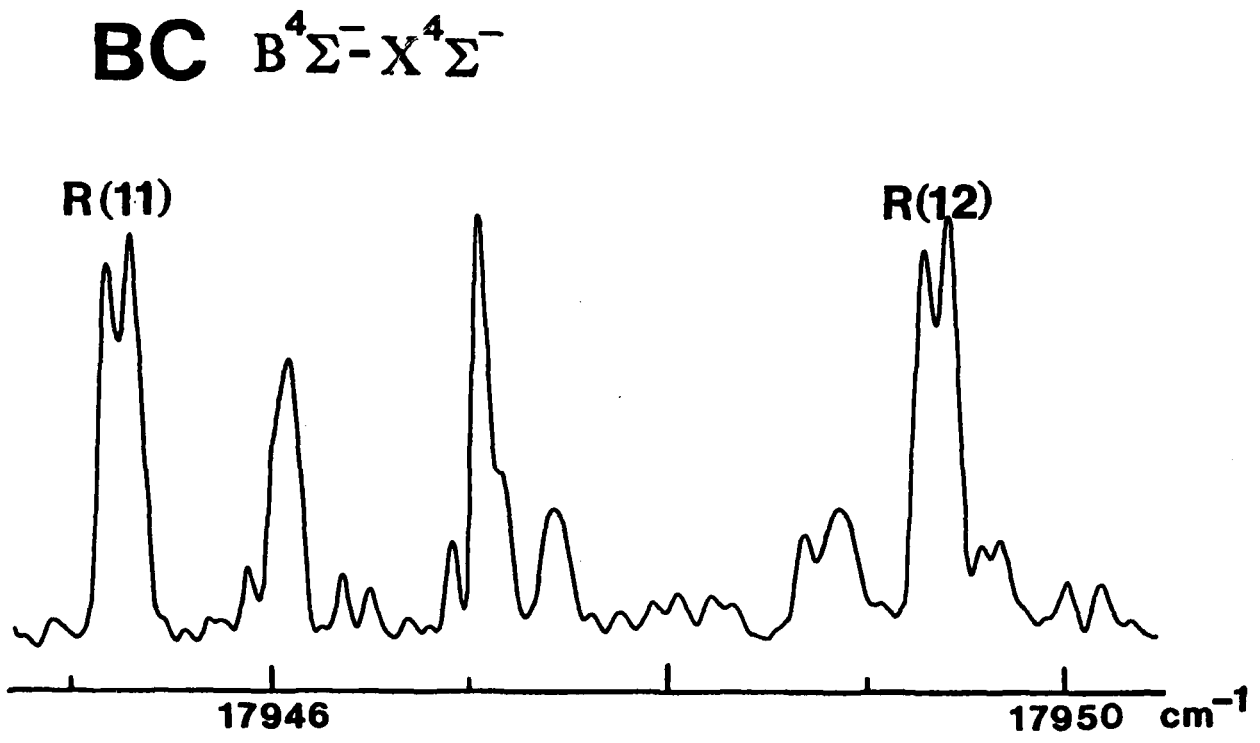

FIGURE 9

Two R branch transitions of the 0-0 band of the $B^4\Sigma^- - X^4\Sigma^-$ transition of BC. Note the spin-splitting in the R(11) and R(12) lines.

I. Dicarbon Nitride, CCN

The ultracold emission spectrum of CCN was observed with an Engelking-type [Engelking, *Rev. Sci. Instrum.* **57**, 2274 (1986)] free radical jet expansion source.[12] The precursor diazoacetonitrile $HC(N_2)CN$ was seeded in He and discharged to provide CCN. The observation[11] of the 000-000, 000-001, 000-002 and 000-100 vibronic bands of the $\tilde{A}^2\Delta$ - $\tilde{X}^2\Pi$ transition allowed the accurate determination of the ν_1 = 1923.2602(74), ν_3 = 1050.7586(12) and $2\nu_3$ = 2094.8153(16) cm^{-1} vibrational modes. The very precise wavenumber scale of the Fourier transform spectrometer allows these infrared active vibrational modes to be determined from an electronic emission spectrum.

J. Metal Borohydrides, $CaBH_4$ and $SrBH_4$

Ca and Sr vapors react spontaneously with diborane (B_2H_6) to give the $CaBH_4$ and $SrBH_4$ free radicals.[13] The Ca or Sr metal was vaporized from a resistively heated crucible, carried to the reaction zone with argon carrier gas, and reacted with diborane. The diborane was held at -130 °C with a pentane/liquid N_2 bath and added as a gas to the Broida oven. The pressures were approximately 1 Torr of argon and 0.035 Torr of diborane. We have detected the $\tilde{B}^2E$ - $\tilde{X}^2A_1$ and $\tilde{A}^2A_1$ - $\tilde{X}^2A_1$ electronic transitions by low resolution laser-induced fluorescence. These molecules are the first metal borohydrides to be detected in the gas-phase.

K. Conclusion and Future Directions

The techniques of high-resolution laser and, particularly, Fourier transform spectroscopy are able to characterize unusual energetic molecules suitable as propellants. These molecules can be made by a variety of chemical and physical processes in electrical discharges and chemical reactors.

The performance of a propellant depends both on the reaction endothermicity and the molecular weight of the product molecules. Light elements are most suitable so the first row elements, Li through Ne, as well as Mg and Al, are most suitable. Light new molecules such as LiB, LiC, $LiNH_2$, etc., are of potential interest.

The first step in this work is the discovery and spectroscopic identification of new molecules. Ultimately these light, energetic molecules must be synthesized efficiently and trapped in condensed phases to make a viable propellant. The work reported here concentrates on the initial phase of the development of advanced propellants.

L. Publications (Supported by F04611-87-K-0020)

1. C.R. Brazier, P.F. Bernath, J.B. Burkholder and C.J. Howard, Fourier Transform Spectroscopy of the ν_3 Band of the N_3 Radical, *J. Chem. Phys.* **89**, 1762 (1988).
2. P.F. Bernath, S.A. Rogers, L.C. O'Brien, C.R. Brazier and A.D. McLean, Theoretical Predictions and Experimental Detection of the SiC Molecule, *Phys. Rev. Lett.* **60**, 197-199 (1988).

3. C.R. Brazier, L.C. O'Brien and P.F. Bernath, The $A^3\Sigma^-$ - $X^3\Pi$ Transition of the SiC Radical, *J. Chem. Phys.* **91**, 7384-7386 (1989).

4. M. Douay, R. Nietmann and P.F. Bernath, The Discovery of Two New Infrared Electronic Transitions of C_2: $B^1\Delta_g$ - $A^1\Pi_u$ and $B'^1\Sigma_g^+$ - $A^1\Pi_u$, *J. Mol. Spectrosc.* **131**, 261-271 (1988).

5. M. Douay, R. Nietmann and P.F. Bernath, New Observations of the $A^1\Pi_u$ - $X^1\Sigma_g^+$ Transition (Phillips System) of C_2, *J. Mol. Spectrosc.* **131**, 250-260 (1988).

6. K.H. Hinkle, J.J. Keady and P.F. Bernath, Detection of C_3 in the Circumstellar Shell of IRC+10216, *Science* **241**, 1319-1322 (1988).

7. P.F. Bernath, K.H. Hinkle and J.J. Keady, Detection of C_5 in the Circumstellar Shell of IRC+10216, *Science* **244**, 562-564 (1989).

8. S.A. Rogers, C.R. Brazier and P.F. Bernath, Fourier Transform Spectroscopy of the $b^3\Pi_g$ - $a^3\Sigma_u^+$ Transition of He_2, *Mol. Phys.* **63**, 901-908 (1988).

9. M. Douay, S.A. Rogers and P.F. Bernath, Infrared Fourier Transform Spectroscopy of XeH, *Mol. Phys.* **64**, 425-436 (1988).

10. F.S. Pianalto, L.C. O'Brien, P.C. Keller and P.F. Bernath, Vibration-Rotation Spectrum of BH $X^1\Sigma^+$ by Fourier Transform Emission Spectroscopy, *J. Mol. Spectrosc.* **129**, 348-353 (1988).

11. A.M.R.P. Fernando and P.F. Bernath, in preparation.

12. N. Oliphant, A. Lee, P.F. Bernath and C.R. Brazier, Fourier Transform Emission Spectroscopy of the Jet-Cooled CCN Free Radical, *J. Chem. Phys.* **92**, 2244-2247 (1990).

13. F.S. Pianalto, A.M.R.P. Bopegedera, W.T.M.L. Fernando, R. Hailey, L.C. O'Brien, C. Brazier, P.C. Keller and P.F. Bernath, in press, *J. Am. Chem. Soc.*