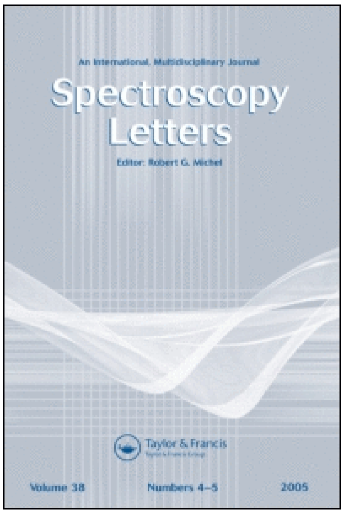

Spectroscopy Letters
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713597299

The $C^1\,\Pi_g$-$A^1\,\Pi_u$ Emission Spectrum of $^{12}C^{13}C$

A. Antić-jovanović[a]; V. Bojović[a]; D. S. Pešić[b]; S. Weniger[c]
[a] Institute of Physical Chemistry, Faculty of Science, University of Belgrade, Belgrade, Yugoslavia [b] B. Kidriĉ Institute of Nuclear Sciences, Belgrade, Yugoslavia [c] Observatoire de Paris, Section d'Astrophysique, Meudon, France

To cite this Article Antić-jovanović, A. , Bojović, V. , Pešić, D. S. and Weniger, S.(1985) 'The $C^1\,\Pi_g$-$A^1\,\Pi_u$ Emission Spectrum of $^{12}C^{13}C$', Spectroscopy Letters, 18: 7, 497 — 506

To link to this Article: DOI: 10.1080/00387018508062250

URL: http://dx.doi.org/10.1080/00387018508062250

SPECTROSCOPY LETTERS, 18(7), 497-506 (1985)

THE $C^1\Pi_g$-$A^1\Pi_u$ EMISSION SPECTRUM OF $^{12}C^{13}C$

KEY WORDS: rotational analysis, isotope shifts, the $^{12}C^{13}C$ molecule

A. Antić-Jovanović and V. Bojović
Institute of Physical Chemistry, Faculty of Science,
University of Belgrade, Belgrade, Yugoslavia

D. S. Pešić
B. Kidrič Institute of Nuclear Sciences, POB 522,
Belgrade, Yugoslavia

and

S. Weniger
Observatoire de Paris, Section d'Astrophysique,
92190 Meudon, France

ABSTRACT

A few bands of the $C^1\Pi_g$-$A^1\Pi_u$ system of $^{12}C^{13}C$ molecule have been photographed and five of them have been rotationally analyzed. Molecular constants for v = 0, 1 and 2 in the $C^1\Pi_g$ and in $A^1\Pi_u$ states have been

0038-7010/85/1807-0497$3.50/0

obtained using a nonlinear least-squares procedure in which all analyzed bands were fitted simultaneosly.

INTRODUCTION

The estimates of relative abundances of isotopes in stellar atmospheres are generally provided by spectrophotometric measurements of molecular spectra. Absorption spectra of cool carbon stars (R and N-types) show isotopic bands involving ^{12}C and ^{13}C whose intensities are use to evaluate reliable isotopic ratios $^{12}C/^{13}C$.

Laboratory high-resolution work on the $C^1\Pi_g - A^1\Pi_u$ system (Deslandres-d'Azambuja bands) of $^{12}C^{13}C$ molecule in the wavelength range between 300 and 420 nm is at now not available. To our knowledge the reported data[1] deal with low resolution bandheads measurements only.

The purpose of the present study is to give results on the rotational analysis of obtained $^{12}C^{13}C$ bands together with evaluated molecular constants for this isotopic molecule.

EXPERIMENTAL

The conditions for obtaining $^{12}C^{13}C$ bands were similar to those described in previous work[2] with the exception that in the experiments reported here, a mixture of helium and acetylene (10:1) containing ^{13}C enriched up to 50% was used.

The bands were photographed on Ilford HP5 emulsion in the 1st order of a 6.4 m Ebert spectrograph with reciprocal dispersion of 0.12 nm/mm. Exposures of 2 - 4 hr were required to record bands with a reasonable good intensity. Iron lines from a hollow cathode discharge were used as a reference spectrum. The line position measurements were converted to vacuum wavenumbers using a high polynomial computer program. The accuracy for unblended lines was about 0.05 cm^{-1}.

ANALYSIS AND RESULTS

In addition to the $^{12}C_2$ and $^{13}C_2$ bands, the following $^{12}C^{13}C$ bands have been obtained: the 0-1, 1-2, 0-0, 1-0, 2-1 and 3-2 bands. Their vibrational assignment, supported by observed isotope shifts, was straightward. Table 1 gives the positions of measured bandheads along with observed isotope displacements $\Delta\upsilon_{obs.}$ and those calculated $\Delta\upsilon_{cal.}$ as the sum of the vibrational and rotational isotope effects using the known isotopic relations[3], the corresponding constants for $^{12}C_2$ (listed in Ref. 4) and $\rho = 0.98052$. The electronic isotope shift is assumed to be zero.

TABLE 1

Bandheads of $^{12}C^{13}C$ and Their Isotope Shifts (in cm^{-1})

$v'-v''$	ν_h	$\Delta\nu_{obs.}$	$\Delta\nu_{cal.}$
0 - 1	24398.75	+29.07	+29.08
1 - 2	24599.30	+24.94	+25.23
0 - 0	25950.70	- 1.50	- 1.24
1 - 0	27679.25	-34.57	-34.39
2 - 1	27790.90	-33.74	-33.99
3 - 2	27837.2	-28.6	-29.8

The band belonging to the $\Delta v = \pm 1$ sequences are sufficiently free from overlapping structure of the $^{12}C_2$ and $^{13}C_2$ bands and all could be analyzed except the 3-2 band which was too weak. The lines of the 0-0 band of the $^{12}C^{13}C$ molecule could also be identified in spite of partial overlapping by the lines of the other two isotopes which were of smaller intensities.

The structure of the bands is consistent with a $^1\Pi-^1\Pi$ transition for heteronuclear molecules with unresolved Λ-doubling. The bands consist of single P and R lines which could be followed with certainty up to J about 15. The Q lines were too faint to be observed.

The J numbering of the lines was carried out by the computer program elsewhere used[2] and was checked by means of second combination differences. Assigned rotational lines are given in Table 2.

Another computer program[5], which fits the experimental wavenumbers to calculated values found by diagonalizing upper and lower states Hamiltonien matrices, was used to derive molecular constants for the $^{12}C^{13}C$ molecule. In the calculating procedure the rotational term expresion of the simple form

$$F_v(J) = B_v[J(J+1)-1] - D_v[J(J+1)-1]^2$$

was used for two $^1\Pi$ state involved in transition since no Λ-doubling is seen. Initial values of molecular constants employed for the calculation were derived from the corresponding constants of $^{12}C_2$ listed in Ref. 6, 7.

Since some of the bands have states in common, the lines of all analyzed bands were fitted simultaneously to dertmine the rotational constants for each vibrational level and the origin for each band. The centrifugal distorsion constants $D_e' = 6.3\times10^{-6}$ cm^{-1} and $D_e'' = 5.9\times10^{-6}$ cm^{-1} (estimated from isotope relations) were kept constant in the fitting procedure. Altogether 140 lines were fitted with a standard deviation the order of magnitude 0.05 cm^{-1}, and in second fit, after removal poorly measured lines, the rotational constants and band origins, given in Tabel 3, were obtained.

TABLE 2

Wavenumbers and Rotational assignments for Bands of the $C^1\Pi_g$-$A^1\Pi_u$ System of $^{13}C^{13}C$ (in cm^{-1})

J	0-1 band				1-2 band			
	P(*J*)	*o*-*c*†	*R*(*J*)	*o*-*c*	*P*(*J*)	*o*-*c*	*F*(*J*)	*o*-*c*
1			24420.77	(0)			24621.50	(+6)
2	24407.80	(-3)	424.90	(+1)	24608.65	(0)	625.50	(+3)
3	405.50	(+3)	429.40	(+4)	606.28	(-2)	629.83	(-2)
4	403.40	(-7)	434.20	(+2)	604.25	(-3)	634.40*	(-15)
5	401.76	(-6)	439.45	(+10)	602.60	(0)	639.70	(+10)
6	400.45	(-7)	444.95	(+9)	601.25	(-1)	645.10*	(+12)
7	399.53	(-4)	450.80	(+7)	600.25	(0)	650.50*	(-17)
8	399.10*	(-12)	456.95	(+1)	599.50	(-8)	656.86*	(+14)
9	398.75	(+2)	463.50	(0)	599.32	(-8)	663.13	(+2)
10	398.75	(-8)	470.40	(0)	599.32	(-8)	669.90	(+9)
11	399.40*	(-11)	477.60	(-5)	599.50	(-8)		
12	400.29*	(-12)	485.40*	(+12)	600.25	(0)		
13	401.17	(-6)			601.25	(0)		
14	402.72	(-1)			602.50	(-8)		
15	404.70*	(+12)			604.25	(+1)		
16	406.82	(+6)			606.28	(+5)		
17	409.04*	(-11)						
18	412.11	(-5)						
19	415.32	(-5)						
20	419.01	(+8)						

TABLE 2 - Continued

J	0-0 band				1-0 band			
	P(J)	o–c	R(J)		P(J)	o–c	R(J)	o–c
1			25974.40	(+3)				
2	25961.40	(+4)	978.48	(+6)			27709.30	(0)
3	959.00	(+9)	982.78	(-2)			713.40	(-8)
4	956.90*	(+12)	987.55	(+6)	27687.70	(+4)	717.38	(+5)
5	955.02	(+5)	992.50	(+1)	685.70	(+5)	722.60	(-5)
6	953.40	(-7)	997.80	(-2)	684.00	(+8)	727.64	(0)
7	952.30	(0)	26003.40	(-6)	682.50	(+4)	733.00	(+10)
8	951.40	(-5)	009.35	(-7)	681.28	(+1)	738.38	(-4)
9	950.70*	(-18)	015.60	(+9)	680.40	(+5)	744.20	(-1)
10	950.70	(0)	022.15*	(+12)	679.70	(0)	750.30	(+3)
11	950.70	(-10)	029.10	(-7)	679.25	(-7)	756.30*	(-28)
12	951.34*	(+12)			679.25	(+4)	763.30*	(+12)
13	951.97	(+2)			679.25*	(+11)	769.98	(-4)
14	953.000	(0)			679.75	(-4)		
15	954.35	(-1)			680.54	(+6)		
16	956.10	(+7)			681.40	(+3)		
17	958.00	(-1)						
18	960.35	(+14)						

(continued)

TABLE 2 - Continued

J	2-1 banc			
	P(*J*)	*o-c*	*R*(*J*)	*o-c*
1			27818.24	(+2)
2			822.08	(+6)
3	27802.94	(+2)	826.04	(+3)
4	800.60	(0)	830.33	(+3)
5	798.50	(-3)	834.81	(-9)
6	769.72	(+1)	839.60	(-8)
7	795.13	(0)	844.64	(-7)
8	793.79	(-1)	849.90	(-8)
9	792.79	(+7)		
10	791.90	(+3)		
11	791.29	(+1)		
12	791.00	(+7)		
13	791.00*	(+18)		
14	791.00	(+5)		
15	791.29	(-4)		
16	791.90	(-4)		

[†] *o-c* denotes observed minus calculated wavenumber in units of 10^{-2} cm^{-1}.

[*] denotes lines which have not been used in the evaluation of the molecular constants.

TABLE 3

Rotational Constants and Band Origins (in cm^{-1})

v	B'_v	B''_v
0	1.7064 (4)*	1.5463 (3)
1	1.6823 (3)	1.5303 (3)
2	1.6539 (4)	1.5139 (4)

υ_{o-1} = 24413.60 (1)
υ_{1-2} = 24614.37 (2)
υ_{o-o} = 25967.23 (1)
υ_{1-0} = 27698.39 (3)
υ_{2-1} = 27811.36 (1)

*The numbers in parenthesis are the uncerainty in the last digits that correspond to standard deviation.

Due to the small number observed bands in v' - and v'' - progressions, the determination of vibrational constants in both involved electronic states was impossible. According to the band origins listed in Table 3, the vibrational quanta are

$$\text{for } C^1\Pi_g \text{ state: } \Delta G_{1/2} = 1731.16 \text{ cm}^{-1}$$

and

$$\text{for } A^1\Pi_u \text{ state: } \Delta G_{1/2} = 1553.63 \text{ cm}^{-1}.$$

ACKNOWLEDGEMENT

We are greately indebted to Dr. C. Amiot (Laboratoire de Physique Moleculaire et d'Optique Atmospherique-Orsay, France) for assistance in using his computer program for analysis of bands. The study was partially supported by the Research Council of Serbia.

REFERENCES

1. H. Cisak, K. Dabrowska and M. Rytel, Acta Phys. Polon. 36,497 (1969).
2. A. Antić-Jovanović, V.Bojović, D. S. Pešić, B.R. Vujisić, D. Rakotoarijimy and S. Weniger, J. Mol. Spectrosc. (in press).
3. G. Herzberg, "Spectra of Diatomic Molecules" p. 169 2nd Ed., Van Nostrand, New York, 1965.
4. K. P. Huber and G. Herzberg, "Constants of Diatomic Molecules", p. 112, Van Nostrand, New York, 1979.
5. C. Amiot, Astrophys. J. Suppl. Seies 52,329 (1983).
6. J. G. Phillips, Astrophys. J. 108.434 (1948).
7. G.Herzberg and R. B. Sutton, Canad. J. Phys. 18,74 (1939).

Received: 03/08/85
Accepted: 04/12/85