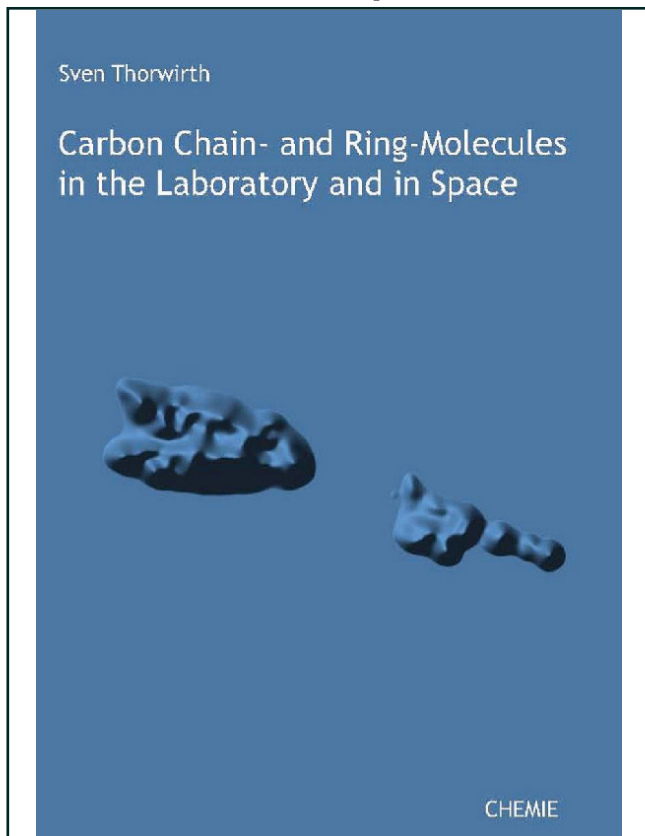




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## **Carbon Chain- and Ring-Molecules in the Laboratory and in Space**



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# 1

## Introduction

Ever since the first detection of atomic and molecular spectral line features in space, secure identifications and proper kinematical analyses have been greatly dependent on the knowledge of accurate laboratory frequencies. So far, approximately 120 molecular carriers have been identified undoubtedly (see Table 1.1 or <http://www.ph1.uni-koeln.de/vorhersagen/molecules/> for an online version) ranging from a variety of light diatomics up to the carbon chain molecule HC<sub>11</sub>N, which is the heaviest molecule detected in space so far [Bell et al. 1997]. Traditionally, laboratory spectroscopy and radio astronomy are concerned with the frequency regime up to approximately 300 GHz corresponding to a wavelength of 1 mm. However, sophisticated techniques have been developed in the last ten years to make the submillimeter-wave range accessible routinely both for laboratory spectroscopy and radio astronomy.

In the laboratory, these techniques are primarily based on high-frequency backward wave oscillators (BWOs, e.g. [Winnewisser et al. 1994], [Winnewisser 1995], [Petkie et al. 1997], [Lewen et al. 1998], [Albert et al. 1998]), on the multiplication of lower frequency Gunn diodes and BWOs (e.g. [Maiwald et al. 1999], [Maiwald et al. 2000]), or on mixing millimeter wave radiation with a THz laser beam to make use of the resulting sideband radiation (e.g. [Lewen et al. 1997], [Gendriesch et al. 2000]). Employing these techniques, spectroscopic investigations can be carried out in the entire frequency regime up to approximately 2.1 THz (70 cm<sup>-1</sup>) covering the fields of pure rotational spectroscopy and rotation-vibration spectroscopy of low-energy vibrational modes (e.g. the  $\nu_2$  mode of C<sub>3</sub> [Giesen et al. 2001]).

In analogy to laboratory spectroscopy, the improvements in receiver development have enlarged the frequency regime accessible to radio telescopes with the construction of high-altitude facilities such as the Kölner Observatorium für Submillimeter Astronomie, KOSMA, on Gornergrat, Switzerland, the Caltech Submillimeter Observatory, CSO, on Mauna Kea, Hawaii, the Heinrich-Hertz-Telescope, HHT, on Mt. Graham, Arizona, or space-borne facilities like the Submillimeter-Wave Astronomy Satellite, SWAS. Future projects such as the Submillimeter Array, SMA, on Mauna Kea, the Atacama Large Millimeter Array, ALMA, Atacama desert, the Herschel Space Telescope, or the airborne Stratospheric Observatory for Infrared Astronomy,

Table 1.1: Interstellar and circumstellar molecules (as of 05/2001).

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms
H <sub>2</sub>	C <sub>3</sub>	c-C <sub>3</sub> H	C <sub>5</sub>	C <sub>5</sub> H	C <sub>6</sub> H
AlF	C <sub>2</sub> H	l-C <sub>3</sub> H	C <sub>4</sub> H	C <sub>5</sub> O	CH <sub>2</sub> CHCN
AlCl	C <sub>2</sub> O	C <sub>3</sub> N	C <sub>4</sub> Si	C <sub>2</sub> H <sub>4</sub>	CH <sub>3</sub> C <sub>2</sub> H
C <sub>2</sub>	C <sub>2</sub> S	C <sub>3</sub> O	l-C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> CN	HC <sub>5</sub> N
CH	CH <sub>2</sub>	C <sub>3</sub> S	c-C <sub>3</sub> H <sub>2</sub>	CH <sub>3</sub> NC	HCOCH <sub>3</sub>
CH <sup>+</sup>	HCN	C <sub>2</sub> H <sub>2</sub>	CH <sub>2</sub> CN	CH <sub>3</sub> OH	NH <sub>2</sub> CH <sub>3</sub>
CN	HCO	HCCN	CH <sub>4</sub>	CH <sub>3</sub> SH	c-C <sub>2</sub> H <sub>4</sub> O
CO	HCO <sup>+</sup>	HCNH <sup>+</sup>	HC <sub>3</sub> N	HC <sub>3</sub> NH <sup>+</sup>	
CO <sup>+</sup>	HCS <sup>+</sup>	HNCO	HC <sub>2</sub> NC	HC <sub>2</sub> CHO	
CP	HOC <sup>+</sup>	HNCS	HCOOH	HCONH <sub>2</sub>	
CSi	H <sub>2</sub> O	HOCO <sup>+</sup>	H <sub>2</sub> CHN	l-H <sub>2</sub> C <sub>4</sub>	
HCl	H <sub>2</sub> S	H <sub>2</sub> CO	H <sub>2</sub> C <sub>2</sub> O	C <sub>5</sub> N	
KCl	HNC	H <sub>2</sub> CN	H <sub>2</sub> NCN		
NH	HNO	H <sub>2</sub> CS	HNC <sub>3</sub>		
NO	MgCN	H <sub>3</sub> O <sup>+</sup>	SiH <sub>4</sub>		
NS	MgNC	NH <sub>3</sub>	H <sub>2</sub> COH <sup>+</sup>		
NaCl	N <sub>2</sub> H <sup>+</sup>	c-SiC <sub>3</sub>			
OH	N <sub>2</sub> O				
PN	NaCN				
SO	OCS				
SO <sup>+</sup>	SO <sub>2</sub>				
SiN	c-SiC <sub>2</sub>				
SiO	CO <sub>2</sub>				
SiS	NH <sub>2</sub>				
CS	H <sub>3</sub> <sup>+</sup>				
HF	SiCN				
SH					
8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	13 atoms
CH <sub>3</sub> C <sub>3</sub> N	CH <sub>3</sub> C <sub>4</sub> H	(CH <sub>3</sub> ) <sub>2</sub> CO	HC <sub>9</sub> N	c-C <sub>6</sub> H <sub>6</sub>	HC <sub>11</sub> N
HCOOCH <sub>3</sub>	CH <sub>3</sub> CH <sub>2</sub> CN				
CH <sub>3</sub> COOH	(CH <sub>3</sub> ) <sub>2</sub> O				
C <sub>7</sub> H	CH <sub>3</sub> CH <sub>2</sub> OH				
H <sub>2</sub> C <sub>6</sub>	HC <sub>7</sub> N				
CH <sub>2</sub> OHCHO	C <sub>8</sub> H				

SOFIA, will further enlarge the frequency regime toward higher frequencies requiring accurate laboratory data in the submillimeter-wave and Terahertz ranges.

A closer look at Table 1.1 reveals, that carbon chain molecules constitute a dominant fraction of the reported interstellar and circumstellar molecules and have drawn much attention in terms of the substantial number of laboratory investigations (e.g. [McCarthy 2000] and references therein). The cyanopolynes,  $\text{HC}_n\text{N}$  ( $n = 1, 3, 5, 7, \dots$ ) are extraordinarily prominent amongst the carbon chains. The shorter members HCN,  $\text{HC}_3\text{N}$  and  $\text{HC}_5\text{N}$  are abundant in a large variety of astronomical sources ranging from quiescent dark clouds with no apparent sign of recent star formation over star-forming regions to circumstellar shells of late type stars (e.g. [Winnewisser and Walmsley 1979]). Due to low-lying bending modes, the molecules cannot only be found in the ground vibrational but also in excited vibrational states in warm regions of the interstellar and circumstellar media (e.g. [Clark et al. 1976], [Ziurys and Turner 1986], [Wyrowski et al. 1999], [Schilke et al. 2000]). The observation of vibrational satellites of carbon chains is a unique probe of hot gas around stars or young stellar objects.

Star-forming regions respectively hot molecular cloud cores are a very challenging class of astronomical objects. They are known to show spectral features due to a multitude of different molecules including relatively complex organics (e.g. [Nummelin et al. 1998a], [Schilke et al. 2001]). This also holds for late type stars, that have been proven to be very rich in terms of molecular line emission as well (e.g. [Bujarrabal et al. 1988], [Cernicharo et al. 2000a]). Therefore, it is necessary to provide constantly accurate laboratory data of molecules to permit the assignment of spectral features in astronomical objects.

In this context, it is the aim of the present thesis to serve the entire field twofold:

The first part is dedicated to pure rotational spectroscopic techniques that have been applied to selected molecules of astrophysical importance. Recently, it has been shown by [Wyrowski et al. 1999] that cyanoacetylene,  $\text{HC}_3\text{N}$ , can be found in highly vibrationally excited states in star-forming regions. This underlines the importance of  $\text{HC}_3\text{N}$  as a probe for highly excited gas in interstellar clouds and circumstellar shells, infrared fields (radiative excitation of vibrational levels), and deeply embedded, luminous infrared objects which are prime targets for high spatial resolution studies. To provide accurate laboratory data in the submillimeter-wave range, the pure rotational spectrum of  $\text{HC}_3\text{N}$  has been measured in the ground vibrational and excited vibrational states up to 814 GHz. Moreover, [Wyrowski et al. 1999] detected vibrational satellites due to  $\text{HC}_3\text{N}$ -isotopomers in space for the first time. In this case, there has been a striking lack of accurate laboratory data to date. Therefore, the pure rotational spectra of monosubstituted  $^{13}\text{C}$ - and  $^{15}\text{N}$ -isotopomers have been measured in the ground vibrational and several vibrationally excited states up to 625 GHz. In addition, the pure rotational spectra of the doubly substituted isotopomers  $\text{HC}^{13}\text{C}^{13}\text{CN}$ ,  $\text{H}^{13}\text{CC}^{13}\text{CN}$ ,  $\text{H}^{13}\text{C}^{13}\text{CCN}$ , and  $\text{HCC}^{13}\text{C}^{15}\text{N}$  have been measured for the first time, not only in the ground but also in vibrationally excited states. Additional measurements were carried out for the isomeric pair HCN/HNC which is widespread in the interstel-

lar and circumstellar media. Selected direct  $\ell$ -type ( $\Delta J = 0$ ) transitions were measured in the millimeter wave regime for HCN. HNC was investigated in the ground vibrational state and first excited bending mode up to 2 THz leading to a set of greatly improved molecular constants. Finally, the millimeter- and submillimeter-wave spectrum as well as the dipole moment of the supposed hot core constituent ethylenimine were measured. The extensive new data set enables accurate predictions of transition frequencies and line intensities that are essential for the unequivocal detection of this molecule in space.

The second part of this thesis is dedicated to astronomical observations which have been performed toward the protoplanetary nebula CRL 618. Protoplanetary nebulae represent a short transition state in the development of late type stars after having left the asymptotic giant branch and evolving towards the planetary nebula phase (e.g. [Kwok 1993]). To derive more information about the physical and chemical conditions in this short-lived evolutionary stage from an observational point of view, the molecules HCN,  $\text{HC}_3\text{N}$  along with two of its isotopomers ( $\text{HCC}^{13}\text{CN}$  and  $\text{HC}^{13}\text{CCN}$ ) and  $\text{HC}_5\text{N}$  have been observed in CRL 618 at radio wavelengths. The observations of HCN resulted in the first detection of direct  $\ell$ -type transitions of any molecule in space. Moreover, direct  $\ell$ -type transitions could be found in the star-forming regions Sgr B2(N), Orion-KL and G10.47+0.03 pointing towards the significance of HCN as a tracer for warm gas in the interstellar/circumstellar media.  $\text{HC}_3\text{N}$  was observed toward CRL 618 in a plethora of vibrationally excited states obtaining information about the temperature structure of the circumstellar envelope. Finally, vibrational satellites of  $\text{HC}_5\text{N}$  in its two lowest lying vibrational states could be found in CRL 618 which stands for the first detection of vibrationally excited  $\text{HC}_5\text{N}$  in space.

The outline of the present thesis is as follows:

The first part “Laboratory Spectroscopy” is opened by Chapter 2 giving an introduction to the spectrometers that have been employed in the present laboratory investigations. Theoretical fundamentals related to rotational spectroscopy will be discussed briefly in Chapter 3. Subsequently, the results obtained for the carbon chain molecules  $\text{HC}_3\text{N}$  (Chapter 4) and several of its isotopomers (Chapter 5), HNC (Chapter 6), HCN (Chapter 7) and ethylenimine (Chapter 8) will be presented.

In the second part “Astronomical Observations”, some introductory comments on protoplanetary nebulae and CRL 618 in particular will be given (Chapter 10). Subsequently, the results derived from observations of HCN will be presented (Chapter 11) followed by the results obtained for  $\text{HC}_3\text{N}$  (Chapter 12) and  $\text{HC}_5\text{N}$  (Chapter 13).

Finally, in the third part “Conclusions and Prospects” the results obtained will be summarized and implications concerning future investigations will be discussed.