

## RADIO AND MILLIMETRE OBSERVATIONS OF LESS COMPLEX MOLECULES

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Progress in laboratory and astronomical instrumentation has renewed the already large interest for simple astrophysical molecules. On the laboratory side, one of the most notable advances has been the spectroscopic observation of an increasing number of small reactive molecular species. On the astronomical side, the access to submillimetre wavelengths and the completion of millimetric interferometers and large single-dish telescopes, have allowed the detection of many new molecular species and open the way for detailed studies of the distribution of molecules in interstellar and circumstellar clouds.

### 1)- New molecules in space

The last two years have seen the discovery of an unusually large number of new astrophysical molecules. These include heavy carbon chain molecules (see the review of L. Avery), the first chlorine (HCl) and phosphorus (PN) -bearing molecules (their identification in space is however still tentative: Phillips et al. 1984, Sutton et al. 1985), and, last but not least, several highly reactive species. We focus here on the discovery of these latter and on their significance for astrochemistry.

Surveys of the millimetre spectrum of the most conspicuous molecular sources (SgrB2, OrionKL and IRC+10216), made at Kitt Peak, Holmdel (Cummins, Linke and Thaddeus 1986), Onsala (Johansson et al. 1984) and Owens Valley (Sutton et al. 1985) during the past ten years, have yielded a large number of unidentified millimetre lines. Some of these have attracted the astronomers' attention because of their relative strength, of their close relation with other lines, or because they were observed only in the radical-rich source IRC+10216. Efforts to identify the carriers of these lines through astronomical studies, ab-initio quantum mechanical calculations and laboratory measurements, have proved in many cases successful and have led to the discovery of exotic molecular species.

A good example of the complementarity of the astronomical and laboratory works is given by the discoveries of  $\text{HCS}^+$ ,  $\text{HCO}_2^+$  and  $\text{C}_3\text{H}_2$ . In 1981, Thaddeus, Guélin and Linke have reported the detection in space of three molecular species, unknown in the terrestrial lab. From the pattern and frequency of the observed lines, they were able to derive some of the molecules' structural parameters and to propose for each species one or few possible identifications. On the basis of its inertia moment, the first species was identified with  $\text{HCS}^+$ , a finding soon confirmed in the laboratory (Gudeman et al. 1981). The second was tentatively identified with protonated carbon dioxide,  $\text{HOCO}^+$ . No obvious candidate stood up for the third molecule, the carrier of a line with a frequency of 85.3 GHz, intense in about every molecular source. Several species were considered, among which cyclopropenylidene,  $\text{C}_3\text{H}_2$ . This latter seemed however not very likely because of its cyclic structure.

Confirmation of  $\text{HCO}_2^+$  and the assignment of U85.3 have come recently from the laboratory. Bogey et al. (1984) succeeded in synthesizing  $\text{HCO}_2^+$  and measuring its rotational frequencies; they found those to agree with the astronomically determined values. Thaddeus, Vrtilik and Gottlieb (1985), were able to observe U85.3 in their laboratory and to characterize its carrier as a neutral, organic species, with an even number of H atoms: from its rotational constants, most likely  $\text{C}_3\text{H}_2$ . Thaddeus et al's identification is now confirmed by the observation in the laboratory (Bogey and Destombes 1986) and in space (Kahane et al. 1986) of the isotopically substituted species  $^{13}\text{CC}_2\text{H}_2$  and  $\text{C}_2^{13}\text{CH}_2$ .

The analysis of the rotational spectrum of  $\text{C}_3\text{H}_2$  reveals that this species is also the carrier of U18.3, another strong and widespread interstellar line (Matthews and Irvine 1985). Both the U85.3 data (see below) and the U18.3 data (e.g. Irvine, this symposium) show that the cyclic  $\text{C}_3\text{H}_2$  is abundant in about every dense interstellar cloud. This result is at odds with the previous belief that ring-molecules may be underabundant in space for chemical reasons. A new, more sensitive search for heavier cyclic compounds, such as pyrrole, pyridine and furan, would be most valuable.

Another three-membered ring discovered in space is  $\text{SiC}_2$ . This radical has been known for a long time, from optical observations, to be present in stellar atmospheres. It has recently been identified in the millimetre spectrum of the infrared star IRC+10216 (Thaddeus, Cummins and Linke 1984). Although the astronomical rotational frequencies fell some 3% short of those derived from the infrared laboratory (Michapoulos et al. 1984), the  $\text{C}_{2v}$  symmetry of the molecule and its low inertia moments left little doubt as to the correctness of this identification. Further support for SiCC being the carrier of the astronomical lines has come now from the detection in IRC+10216 of 3 weak lines at the frequencies predicted for  $^{29}\text{SiCC}$  and  $^{30}\text{SiCC}$  (Cernicharo et al. 1986). After SiO, SiS and SiH<sub>4</sub>, SiC<sub>2</sub> is the fourth

silicon-bearing molecule observed in the envelope of this star (a fifth silicon compound may also have been detected, as will be seen below). So far,  $\text{SiC}_2$  has not been seen in any interstellar cloud.

CN and the linear radicals  $\text{C}_3\text{N}$ ,  $\text{C}_2\text{H}$  and  $\text{C}_4\text{H}$  are known to be relatively abundant in sources like IRC+10216 and the dark cloud TMC1.  $\text{C}_2\text{N}$ , whose rotational constant is known from the optical works of Merer and Travis (1965) and Kakimoto and Kasuya (1982), was searched, but not found, implying that the intermediate species  $\text{C}_2\text{N}$ ,  $\text{C}_4\text{N}$ ,  $\text{C}_3\text{H}$  and  $\text{C}_5\text{H}$ , which have an odd number of heavy atoms, are much less abundant. Green (1980) showed however that  $\text{C}_2\text{N}$  has a relatively small dipole moment ( $\approx 1.3$  D), so that the limit set by the searches was not significant; on the other hand, he calculated a large dipole moment (3.1 D) for  $\text{C}_3\text{H}$ , the acetylenic analog of  $\text{C}_2\text{N}$ , showing that this species should be easier to detect in an astronomical source than  $\text{C}_2\text{N}$ . Although no spectroscopic data was available for  $\text{C}_3\text{H}$ , the linear structure calculated by Green provided a rough estimate of this radical's rotational frequencies. This, plus the characteristic  $\Lambda$ -doubling fine structure of the lines, proved sufficient for a tentative identification of the radical in IRC+10216 (Johansson et al. 1984, Thaddeus et al. 1985a), an identification subsequently confirmed in the laboratory (Gottlieb et al. 1985). The relative strength of  $\text{C}_3\text{H}$  in IRC+10216 leads to think that  $\text{C}_5\text{H}$  could also be observed. In fact, this species may already have been detected in that source (see below).

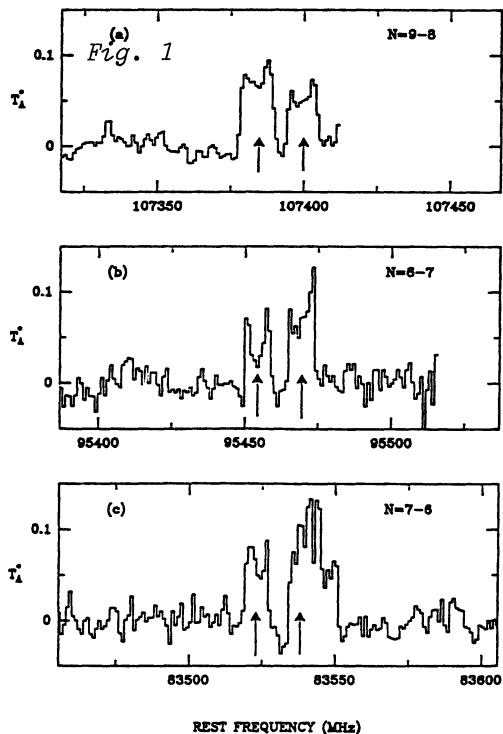
Another carbon-chain molecule detected recently in space is  $\text{C}_3\text{O}$ . This molecule was expected to be abundant in interstellar clouds, as it is isoelectronic with  $\text{HC}_3\text{N}$  and can be formed from CO. Its rotational spectrum has been studied for the first time by Brown et al. (1983) and it has been subsequently detected in TMC1 (Matthews et al. 1984). A fractional abundance  $[\text{C}_3\text{O}]/[\text{H}_2] \approx 1.4 \cdot 10^{-10}$  is derived in that source. As in the cases of  $\text{C}_4\text{H}$  and  $\text{HC}_3\text{N}$ , the abundance of  $\text{C}_3\text{O}$  is lower in the hot giant molecular clouds (Brown et al. 1985).

Protonated hydrogen cyanide,  $\text{HCNH}^+$ , is a likely progenitor of HCN and HNC, and as such has been searched for a long time both in interstellar space and in the laboratory. Detailed IC quantum mechanical calculations of its geometry (Allen, Goddard and Schaefer 1980, Dardi and Dykstra 1980) have confirmed that it has a linear structure and yielded accurate estimates of its moment of inertia; the dipole moment of  $\text{HCNH}^+$  was found to be very small ( $\sim 0.3$  D, Haese and Woods 1979, Lee and Schaefer 1984), ten times smaller than that of HCN, which explains why the microwave rotational spectrum of this species was so difficult to observe. This spectrum has finally been observed in the lab at infrared (Altman, Crofton and Oka 1984) and millimetre (Bogey, Demuyneck and Destombes 1985) wavelengths, and the rotational transition frequencies at last are known well enough for sensitive astronomical searches. Zuirys and Turner (1986) report the probable detection of this ion in an astronomical source, SgrB2.

Phillips et al. (1985) have reported the tentative detection of

$\text{H}_2\text{D}^+$  in NGC2264, a dense and relatively cold molecular cloud.  $\text{H}_2\text{D}^+$ , which is believed to play a key role in the enhancement of molecular hydrides in deuterium (see below), has recently been detected in the spectroscopic laboratory. The frequency of its  $1_{10}-1_{11}$  transition has been accurately measured (Bogey et al. 1984, Warner et al. 1984) making possible the astronomical detection.

Finally, although the  $\text{O}_2$  molecule is still unobserved in astronomical sources, it is worth quoting the recent works of Liszt and Vanden Bout (1985) and Goldsmith et al. (1985), which set limits on the  $\text{O}^{18}\text{O}/\text{C}^{18}\text{O}$  abundance ratio in a few galactic sources. The limit derived in the dark cloud  $\rho\text{-Oph}$  ( $<0.13$ ), which depends, it is true, on excitation conditions, is low enough to set constraints on oxygen chemistry models.



with the Kitt Peak and Onsala telescopes and did not show very many lines. Several of the new U-lines detected with the IRAM telescope appears to form close doublets with harmonically related frequencies; they are not observed in Orion (KL) or SgrB2(OH), which make us think that they arise from linear or quasi-linear radicals.

Figure 1 shows a set of three doublets with centre frequencies almost exactly in the ratios 7/8/9. The doublets have equal splittings and must certainly belong to the same molecule. This latter must be linear or be a slightly asymmetric top, since its rotational frequencies

The completion of larger, new generation telescopes, operating at millimetre and submillimetre wavelengths, will undoubtedly increase the number of known exotic astrophysical molecules and make space a privileged place for the study of highly reactive species. First observations with the 45m Nobeyama telescope uncovered new unidentified lines in the 8mm spectrum of TMC1, the strongest of which, at 45.379 GHz, defies so far identification (Suzuki, this symposium). A recent survey, made with the new 30m IRAM telescope, of a 9 GHz wide band in the 3mm spectrum of IRC+10216, reveals 40 new lines, 30 of which cannot be assigned to any previously known astrophysical molecule (Guélin et al. 1986). This number of new molecular lines is impressive, since this region of the spectrum of IRC+10216 was previously surveyed

fit so exactly an harmonic relation. Its rotational states must be split by spin-rotation interaction and the molecule must have an odd number of electrons: it is thus a radical. From the rotational frequencies, we can determine precisely the rotational constant (5967 MHz) and the moment of inertia of the new radical; it is readily shown that it is most probably composed of one atom of the third-row (sulfur or silicon), two atoms of the second-row (probably carbon or nitrogen) and, possibly, one hydrogen atom. Among the few stable species which fit these conditions, the most probable are  $\text{HSiC}_2$ ,  $\text{NCSi}$  and  $\text{HSC}_2$ . A quantum mechanical study of the ground electronic state of these three species would be needed to determine which one has the proper structure and the right moment of inertia. Five other close doublets, discovered with the IRAM 30m telescope, have centre frequencies in the ratios 17.5/18.5...21.5. They very probably arise from a single linear radical with a  $2\sigma$  ground state; from its moment of inertia, we tentatively identify this radical with  $\text{C}_3\text{H}$  (Cernicharo et al. 1986).

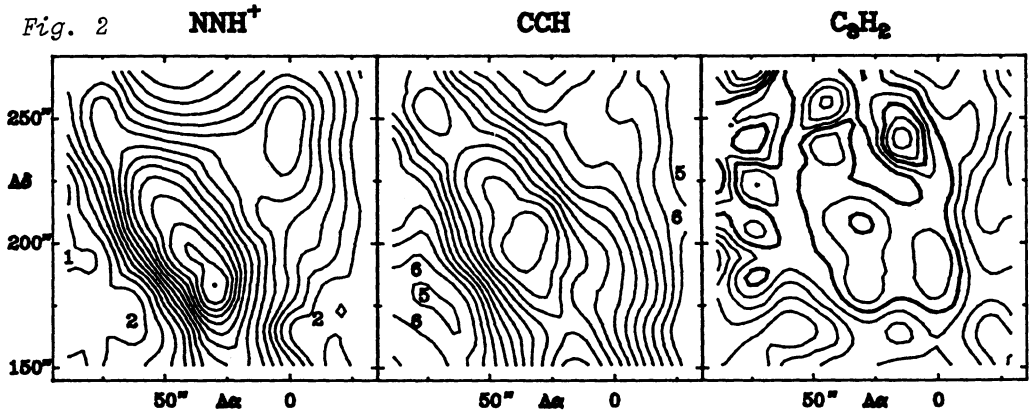
## II) Distribution of molecules in dense clouds

The difference in molecular content between the envelope of IRC+10216 and sources like Orion KL and SgrB2 is certainly not the only one observed between dense clouds. Chemical differentiation was first noticed between the hot giant molecular clouds and the cold quiescent clouds (for example, the  $\text{C}_4\text{H}$  radical is not detected in the hot clouds, but is very abundant in the cold clouds). Other differences have been found between some giant clouds (e.g. Orion KL, which is rich in saturated species, and SgrB2, where unsaturated molecules seem to dominate), as well as between different components of the same clouds (the ridge and the KL nebula in OMC1, Turner and Thaddeus 1977). These chemical differences were at least partly attributed to differences in temperature and density (e.g. Snyder, Watson and Hollis 1977), an explanation which became less convincing when large abundance variations were found between cold clouds with similar physical conditions (e.g. the difference in cyanopolyynes abundance between TMC1 and L134N, Ungerechts, Walmsley and Winnewisser 1980). New, higher resolution observations of molecular lines, made with single-dish telescopes and interferometers, make now clear that molecular abundances also depend on more subtle parameters, linked to the cloud location and its past evolution.

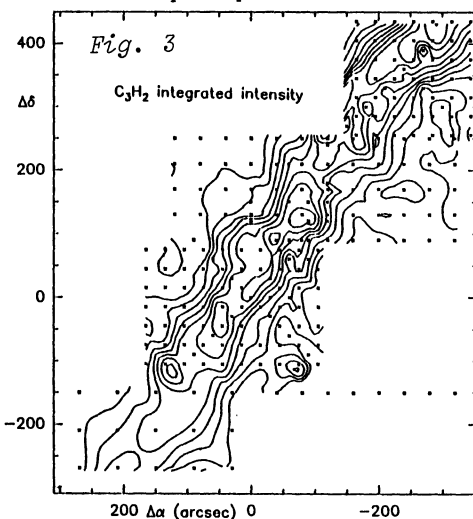
Single dish (Johansson et al. 1984, Wilson et al. 1986) and interferometric (Genzel et al. 1982, Pauls et al. 1983, Wright et al. 1983, Masson et al. 1984) observations of the KL region of OMC1, show that molecules such as  $\text{NH}_3$ ,  $\text{HCN}$ ,  $\text{HCO}^+$ ,  $\text{SO}$ ,  $\text{SO}_2$  and  $\text{CO}$  have different relative abundances in the "spike", the hot core and the "plateau" components. The molecules which are more abundant in the "plateau" could have been predominantly formed in shocked gas (e.g. Mitchell, this symposium). Observations of the northern ridge region in OMC1 show that the emission from several radicals peaks some 3' north of the KL nebula (Turner and Thaddeus, 1977). This northern source has been

studied in the (1,1) and (2,2) transitions of  $\text{NH}_3$  with the Effelsberg 100m telescope (Batra et al. 1983) and with the VLA (Harris et al. 1983). The ammonia inversion lines, which are good probes of the gas temperature and density show that the source consists of two very dense clumps embedded in a less dense and relatively hot cloud. The size of the clumps is  $\approx 10''$ , according to the VLA data; their temperature is  $\approx 40$  K and their density  $10^5 - 10^6 \text{ cm}^{-3}$ .

Fig. 2



The emission from several molecules has recently been mapped in the northern OMC1 source with a  $\approx 25''$  resolution, using the IRAM 30m telescope (Cernicharo, Baudry and Guélin, in preparation).  $\text{N}_2\text{H}^+$ ,  $\text{C}_2\text{H}$  and  $\text{C}_3\text{H}_2$  show different brightness distributions (see Fig 2, where the offsets, in arc second, are relative to IRC2) : the velocity integrated intensity contours of the 1-0  $\text{N}_2\text{H}^+$  line peak on both the SE and the NW ammonia clumps; those of  $\text{C}_2\text{H}$  peak only on the NW clump, while the  $\text{C}_3\text{H}_2$   $2_{12}-1_{01}$  line emission is more or less uniformly distributed. A preliminary analysis of the excitation of the lines shows that the different distributions of Fig.2 reflect true abundance variations. What causes the peculiar molecular composition of the two clumps remains an open question.

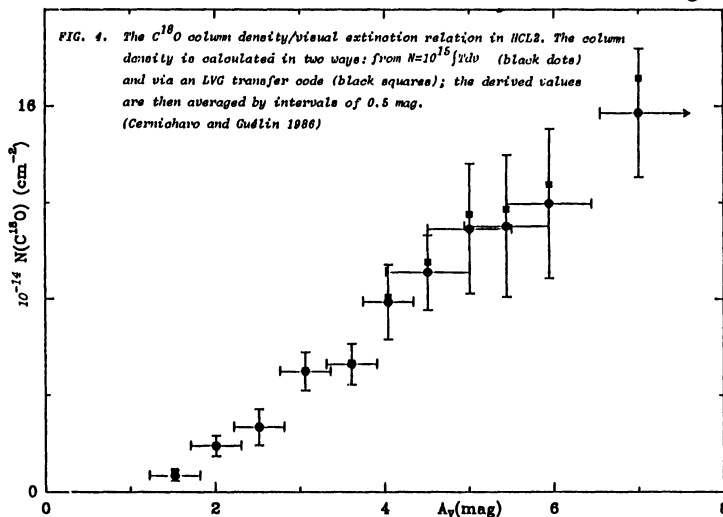


Small and dense clumps with peculiar molecular abundances are not unique to hot clouds like OMC1. They are also found in nearby cool dark clouds such as  $\rho$ -Oph and TMC1. Fig. 3, which presents the velocity integrated intensity contours of the  $\text{C}_3\text{H}_2$   $2_{12}-1_{01}$  line, observed with the IRAM 30m telescope (Cernicharo, Baudry and Guélin, *ibid*), shows that the TMC1 "ridge" is not a thin disk, but a chain of dense clumps of size  $\approx 0.01$  pc. The abundance of heavy cyanopolyynes appears to be larger in the SE clumps, while that of  $\text{NH}_3$ ,  $\text{HCO}^+$

and  $\text{HCS}^+$  seems higher in the NW clumps; line opacity makes however difficult to entangle, in this cold source, the effects of line excitation from those of molecular abundance variations.

Molecular abundances are also expected to vary from the periphery to the centre of the clouds. At the cloud borders, molecules are destroyed by UV radiation; in the cores of cool dense clouds, they may condense on dust grains. Characteristic reaction times between molecules also vary as the gas density increases in the central region. The molecule the best studied in the dense clouds is certainly CO. Except at the border of the clouds, the  $^{12}\text{C}^{16}\text{O}$  and  $^{13}\text{C}^{16}\text{O}$  rotational lines are optically thick, and the CO abundance must be derived from observation of the rarer  $^{12}\text{C}^{18}\text{O}$  isotope (or, whenever they are detectable, of the very rare  $^{12}\text{C}^{17}\text{O}$  and  $^{13}\text{C}^{18}\text{O}$  isotopes), assuming that the abundance of this species, relative to  $^{12}\text{C}^{16}\text{O}$ , is known. At the cloud borders,  $^{12}\text{C}^{18}\text{O}$  is difficult to excite and its abundance may not reflect that of the main isotope, because of isotope-selective photodissociation (e.g. Glassgold, Huggins and Langer 1985); the  $^{12}\text{C}^{16}\text{O}$  or the  $^{13}\text{C}^{16}\text{O}$  lines are there a better tracer of the total CO abundance.

Early  $^{13}\text{C}^{16}\text{O}$  studies and, mostly, the accurate  $^{12}\text{C}^{18}\text{O}$ ,  $^{12}\text{C}^{17}\text{O}$  and  $^{13}\text{C}^{18}\text{O}$  observations of Frerking, Langer and Wilson (1982), made believe that the CO fractional abundance was varying much inside the dark clouds and that it was lower in the densest parts of the clouds. The more thorough studies of Cernicharo and Guélin (1986), Bachiller and Cernicharo (1986) and Duvert, Cernicharo and Baudry (1986), which compare the  $^{12}\text{C}^{18}\text{O}$  column densities in three dark clouds with the visual extinction derived from star counts (as well as with the  $100\mu\text{m}$  emission from dust), on the contrary show no evidence of an abundance variation, except at the very border of the clouds. They yield a common value of the CO fractional abundance in the region  $2 < A_V < 6$ :  $[\text{CO}]/[\text{H}_2] \approx 10^{-4}$  (e.g. Fig.4).



It is true that the decrease of the CO abundance reported by Frerking et al. appears mostly at visual extinctions larger than 6 mag. There are good reasons however to think that the high extinctions they quote are over-estimated: these extinctions are derived from IR photometric measurements in the line of sight to highly reddened IR stars; yet, the

most reddened of these stars fall in areas where star counts indicate only moderate extinction. The large photometric extinctions must thus refer to solid angles much smaller than those used in the star counts or those sustained in the CO observations. As reported by Cernicharo and Guélin (1986), some of the most reddened stars of Frerking et al. coincide with point-like IR sources and are likely to be surrounded by a dust cocoon. This cocoon contributes much to the reddening on the line of sight to the star, but little to the CO intensity, as the latter, observed with a high angular resolution, is not larger toward the star than in adjacent directions.

The region  $A_v < 6$  mag contains typically 95 % of the mass of a dark cloud such as Heiles Cloud 2; it excludes only a few condensations. Evidence that even in these condensations  $[CO]/[H_2]$  is not much smaller than  $10^{-4}$  comes from the high deuterium to hydrogen ratio in high dipole moment hydrides, like  $HCO^+$  and  $N_2H^+$ . As is well known (see e.g. Guélin, Langer and Wilson 1982), these species are enhanced in deuterium inside cold dark clouds by factors of  $\approx 10^3$  with respect to the interstellar atomic deuterium abundance. This enhancement is thought to be caused by deuterium exchange reactions involving HD (as the reaction  $H_3^+ + HD \rightleftharpoons H_2D^+ + H_2$ ) or D (see e.g. Dalgarno and Lepp 1984). If the  $H_2D^+$  recombination rate is very small, as indicated by the measurements of Smith and Adams (1984), the enhancement of  $H_3^+$  in deuterium in cold clouds is limited essentially by the reaction of  $H_2D^+$  with neutrals (probably mostly CO,  $N_2$  and  $H_2O$ ). If  $HCO^+$  and  $N_2H^+$  are mainly formed from  $H_3^+$ ,  $DCO^+/HCO^+$  is at least  $1/3 H_2D^+/H_3^+$ . The observed  $DCO^+/HCO^+$  ratio sets then a limit on  $H_2D^+/H_3^+$ , which in turn yields a lower limit to the abundance of neutrals. In cold clouds the last species to condense on grains are probably CO and  $N_2$ . Since, very probably,  $[CO] > [N_2]$ , we can derive a limit on the CO fractional abundance (and a measure of this abundance if the deuterium enhancement in  $HCO^+$  comes only from  $H_2D^+$ ). In TMC1, as well as in other similarly cold cloudlets, the  $HCO^+/DCO^+$  ratio is found constant and equal to  $\approx 100$  as one deepens into the cloud core (Guélin et al. 1982). This yields  $[CO]/[H_2] > 1-2 \cdot 10^{-4}$ , which means that the depletion of CO is not much larger in the core than in the rest of the cloud.

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#### DISCUSSION

JACKSON: Does the HCN detection in comet Halley agree with the observations of CN radical in comet Halley?

GUÉLIN: I was not part of the team which detected HCN. I do not think they observed CN but I cannot really say.

BLACK: I would like to clarify that the SiC<sub>2</sub> was first identified in the carbon rich envelope, not unlike that of IRC+10° 216, from the optical spectrum about eight years ago. This is distinct from the photospheric feature.

IRVINE: How definitive is your detection of <sup>13</sup>CCH? Is there any laboratory data on this species?

GUÉLIN: Yes, there are some higher frequency microwave measurements by the Lille group but their signal to noise ratio is not good enough to identify definitely the hyperfine components and hence to be able to predict accurately the hyperfine splittings of the 1-0 line. Using

these measurements, and ESR data or matrix-trapped  $^{13}\text{CCH}$ , one nevertheless derives frequencies not incompatible with those we observe in IRC+10216.

HERBST: How can you be sure that the unknown series of doublets derives from a quasi-linear molecule?

GUELIN: We know it derives from a linear or a quasi-linear molecule because of the very good harmonic relation (namely 7/8/9) which exists between the doublet center frequencies. We can in fact get an upper limit of  $3 \times 10^{-7}$  to the molecule asymmetry parameter, which means it has no more than 2 H atoms out of the molecular axis.

K.K. GHOSH: If  $\text{C}_3\text{H}_2$  is a ring molecule, is it a metastable isomer?

GUELIN: The  $\text{C}_3\text{H}_2$  observations reported here refer to the stable three-membered ring. There is another quasi-linear isomer of  $\text{C}_3\text{H}_2$  which may have been observed in SgrB2 by Thaddeus, Vrtilik and Gottlieb (1985).

DEFREES: I have recently completed fairly reliable though not definitive ab initio calculations on isomers of  $\text{C}_3\text{H}_2$ . The three-membered ring, cyclopropenylene, is not a metastable species but the lowest energy isomer. Calculation of rotational frequencies would indicate that the tentative identification of propargylene is incorrect.

P.A. FELDMAN: What is the doublet separation of those three doubles that you attribute to CCNC preliminarily?

GUELIN: It is 15.1. It is pretty well measured even if you have light blending, because all the lines in the source except for maser line like HCN, have exactly the same width in the velocity. And because of that, if you see one edge and know signal to noise ratio, then you know exactly where the centre of the line is. And that trick we had to use for the longest doublet.

HUEBNER: Since we detected HCN in the comet Kohoutek more than ten years ago, there have been many unsuccessful attempts to detect it again in other comets. Therefore, I am very happy that you have detected it. When it was observed in comet Halley? Do you know what the heliocentric distance was and what the column density was for this?

GUELIN: I can tell you the date when it was observed. It was November 20, 1985. I do not want to tell anything more, as it is not my data.