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BOUNDARY CONDITIONS FOR THE PALEOENVIRONMENT: CHEMICAL AND
PHYSICAL PROCESSES IN THE PRE-SOLAR NEBULA

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Current Research

In new observations carried out at the Onsala Space Observatory in Sweden Irvine and Å. Hjalmarsen have succeeded in detecting two additional hyperfine components of the $^2\Pi_{1/2}$, $J=3/2-1/2$, transition of the new interstellar radical C_3H . The results significantly refine earlier estimates of the hyperfine parameters obtained from recent laboratory spectroscopy at Columbia University and earlier astronomical measurements by our group and collaborators at Onsala and the Bell Laboratories. The spectroscopic characterization of this species and the astronomical results will be published shortly (Thaddeus *et al.* 1985). The results provide important data for theories of interstellar chemistry, in which C_3H is a link in various schemes for synthesizing heavier organic molecules (*e.g.*, Millar and Freeman, *MNRAS* 207, 405, 1984).

In previous semi-annual reports we have discussed our continuing investigation of the organic chemistry in the cold, dark interstellar clouds which may be formation sites for solar type stars. These regions have been shown to exhibit a complex chemistry with apparently significant chemical gradients

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within particular clouds and differences among clouds. In observations at the Five College Radio Astronomy Observatory (FCRAO), operated by the University of Massachusetts, we have recently made the first detection of methanol in such regions. Approximately equal abundances were obtained in TMCl and L134N. These 96 GHz observations will be complemented by observations of the lowest rotational transitions at approximately half that frequency, using the facilities of the Onsala Space Observatory in Sweden.

Friberg and Irvine have renewed their search for the radical HCCN, for which laboratory spectroscopic data have recently been obtained in Japan. Observations at FCRAO were carried out for the warm, giant molecular clouds SgrB2 and Orion KL and towards the envelope of the evolved carbon star IRC+10216, complementing our previous search in the cold, dark cloud TMCl (Suzuki et al., 1985). Upper limits were obtained which significantly constrain the abundance of HCCN in these regions. In particular, HCCN is much less abundant than either HCN or HC_3N , in accord with models of interstellar chemistry in which such carbon chains grow primarily by the addition of even units through interaction with acetylene and acetylenic ions. In the process of the search the first astronomical detection was made of b-type transitions of methylformate, towards Orion KL.

In a continuing collaboration with scientists at the Chemistry Department of Monash University in Australia, we have carried out a deep search for keteneimine (H_2CCNH) at the FCRAO. The rotational spectrum was recently measured for the first time in the laboratory by the Monash Group. Ab initio quantum mechanical calculations (deFrees et al., preprint, 1984) had suggested that this isomer of the well known interstellar molecule methylcyanide might be reasonably abundant in molecular clouds. We have shown that this is in fact not the case.

Irvine and UMass graduate students used the National Radio Astronomy Observatory (NRAO) 43 m telescope in Green Bank, West Virginia, to search for another isomer of methylcyanide, HCCNH_2 (aminoacetylene). Since other acetylene derivatives are well known in cold, dark interstellar clouds, our failure to observe aminoacetylene appears to rule out certain theories for the formation of related molecules such as methylacetylene and cyanoacetylene. In the process of these observations, we have apparently detected for the first time emission from a very highly excited, non-metastable state of ammonia ($J,K=9,6$) towards certain warm molecular clouds. The data seem to imply either maser emission or extremely warm, dense condensations, which may be sites of star formation.

As we have discussed in several reviews (e.g., Irvine *et al.*, 1985), the determination of absolute abundances in molecular cloud cores is one of the most challenging problems faced by radio astronomers. Schloerb and colleagues are approaching this problem in a new way, through observations of the 1.3 mm continuum radiation from dust in the cloud cores. They have obtained maps of the cores of the Orion, W49, and W51 molecular clouds in both 1.3 mm continuum emission and the C^{18}O $J=2-1$ line. Since each map reveals an independent tracer of mass column density, the observations permit one to study the effectiveness of each in determining the mass distribution within these cores. Comparison of the C^{18}O intensity, which traces the gas column density, with that of the 1.3 mm continuum intensity, which traces the dust, reveals the expected significant correlation between the two quantities. However, this ratio depends strongly on the gas and dust temperatures, which are not the same in all three sources. A preliminary attempt to correct for temperature effects using the far infrared observations of the grain temperature and ^{12}CO observations of the gas temperature suggest that the maps are consistent with the

nominal values of the extinction efficiency of grains and the CO abundance. This result indicates that large depletion of CO on to grains in the dense cores of molecular clouds probably does not occur.

We have previously pointed out that the relative abundance of chemical isomers such as HCN/HNC, $\text{HCO}^-/\text{HOC}^+$, and $\text{CH}_3\text{CN}/\text{CH}_3\text{NC}$ can place significant constraints on chemical processes in the interstellar medium. Our data have shown that HNC is slightly more abundant than HCN in the cold dark cloud TMCl, and that the abundance ratio can vary significantly in the warmer giant molecular clouds. In an effort to understand the physical and chemical basis for such variations, emission from HNC/HCN was mapped in the Orion molecular cloud by Irvine and Swedish colleagues at the Onsala Observatory. In order to avoid problems of line saturation, observations were made of the ^{13}C and ^{15}N species. Initial reduction of the data shows that significant variations exist between the hot, dense core of the cloud and cooler regions. Very recently additional data have been obtained at FCRAO for more outlying portions of the cloud.

In our last grant proposal we reported the determination of accurate abundance ratios for various cyanide and isocyanide compounds in the cold, dark cloud TMCl, including a tentative first identification of interstellar methyl-isocyanide (CH_3NC). We are encouraged that our observations have stimulated theoretical work on the structure and formation mechanisms of the isomeric pair $\text{CH}_3\text{CN}/\text{CH}_3\text{NC}$ (deFrees *et al.*, preprint, 1984), an effort also supported by the NASA Exobiology Program. In fact the predictions for the abundance of CH_3NC in cold interstellar clouds support our tentative identification.

In collaboration with colleagues at the Onsala Space Observatory in Sweden, the first very broad bandwidth, consistently calibrated spectra for astronomical sources at millimeter wavelengths have been published in atlas form

(Johansson et al., 1984). The results should be extremely useful to all millimeter wavelength radio observatories.

The dense cores in several nearby dark clouds have been probed by mapping in several CO isotopic transitions, to provide fundamental information on the molecular content of these important sources. In addition, the proximity of these clouds permits resolutions close to the sizes predicted for protostars. Cores mapped in C¹⁸O include L134N, B335, and TMC-1. The most extensive map has been made (700 spectra) in TMC-1, revealing a complex structure of condensations, each similar in size and mass to what is expected for low mass protostars. The observations, therefore, suggest that the long filamentary ridge in TMC-1 is in the process of fragmenting into numerous clumps of approximately stellar mass that may eventually form solar-type stars. Interestingly, the comparison of this data to more limited maps obtained in other molecules further suggests that there are apparent chemical differences between these clumps. Further studies of the chemistry of these coevolving fragments may help us to understand whether these apparent differences are real, or are indicative of an extreme sensitivity of the line formation process to physical conditions. In recent observations at the NRAO 43 m telescope we have complemented the FCRAO data described above with limited results on the spatial distribution in L134N of ammonia and cyanoacetylene.

Ziurys, Friberg, and Irvine have undertaken a deep search for silicon monoxide (SiO) in cold, dark clouds. Previous astronomical observations had detected SiO only in regions of massive star formation, particularly in those exhibiting high velocity outflows and high temperatures. Our results to date indicate that in the coldest clouds SiO is depleted by at least an order of magnitude relative to these hotter regions, perhaps indicating the inclusion of silicon into interstellar dust particles. The situation is complicated, however,

since we have finally succeeded in detecting SiO in the outlying portions of the Orion cloud, where star formation is not apparent. These studies will be pursued.

Observations have been performed by Ziurys at the NRAO 12 meter antenna and the 4.9 m. dish of the Millimeter Wave Observatory (U.Texas). One aspect of these studies involves searches for two possible new interstellar ions, HCNH^+ and SH^+ . Although the search for SH^+ was inconclusive, it appears that the $J=1\rightarrow 0$ and $J=2\rightarrow 1$ transitions of HCNH^+ have been seen; in order to securely confirm the detection of this molecule, the $J=3\rightarrow 2$ line must be observed, and this work will be done in the near future. Observations of new molecular ions are important for verification of ion-molecule chemical theory.

A search was also performed for NH_2 , another possible new interstellar molecule. Several lines were detected in this search that may be attributable to NH_2 , and confirming observation time is being awaited.

In addition to searches for new molecular species studies, Ziurys is pursuing known interstellar molecules in excited states. Rotational transitions of HCO^+ , HCN, and HNC in vibrationally-excited states have been searched for. Several lines have been observed towards Orion-KL, the classical source of high excitation, that are coincident in frequency with lines originating in the two stretching modes of HCO^+ . Towards IRC+10216, lines corresponding possibly to the bending mode of HCN have been seen. Confirmation of these transitions will occur this spring. Studies of vibrationally-excited interstellar species reveal a great deal of information concerning excitation conditions in astronomical sources. The $N=4\rightarrow 3$ rotational lines of CCH have also been detected toward the Orion (3N,1E) position. Observations of these lines show that CCH is present at high densities, and are additional evidence for the occurrence of active carbon chemistry in cloud cores.

Results of research supported by this grant were reported at the recent meeting of the American Astronomical Society in January of 1985 by Irvine.

Papers supported by this grant and published during the period of this report:

1. "Confirmation of the Existence of Two New Interstellar Molecules: C_3H and C_3O ", Irvine, W.M., Friberg, P., Hjalmarson, Å., Johansson, L.E.B., Thaddeus, P., Brown, R.D., and Godfrey, P.D., Bull. Amer. Astron. Soc., 16, 877 (1984).
2. "Molecular Structure of L134N", Swade, D.A., Schloerb, F.P., and Snell, R.L., Bull. Amer. Astron. Soc., 16, 937 (1984).

Research supported by this grant currently in press:

1. "The Chemical State of Dense Interstellar Clouds", Irvine, W.M., Schloerb, F.P., Hjalmarson, Å., and Herbst, E., in Protostars and Planets II, ed. D. Black, (University of Arizona Press), in press (1985).
2. "Comets and the Origin of Life", McGunagle, C. and Irvine, W.M., Bulletin Portuguese Chemical Society, in press, (1985).
3. "Recent Observations of Interstellar Molecules in Nearby Cold, Dark Interstellar Clouds", Suzuki, H., Ohishi, M., Morimoto, M., Kaifu, N., Friberg, P., Irvine, W.M., and Matthews, H.E., in Search for Extra-terrestrial Life - Recent Developments, ed. M. Papagiannis (D. Reidel), in press (1985).
4. "The Spectra of Orion A and IRC+10216 between 72.2 and 91.1 GHz", Johansson, L.E.B., Andersson, C., Ellder, J., Friberg, P., Hjalmarson, Å., Hoglund, B., Irvine, W.M., Olofsson, H., and Rydbeck, G., Astron. Astrophys. Suppl., in press (1985).
5. "The Detection of Acetaldehyde in Cold Dust Clouds", Matthews, H.E., Friberg, P., and Irvine, W.M., Astrophys. J., in press (1985).
6. "Search for Molecular Oxygen in Dense Interstellar Clouds", Goldsmith P.F., Snell, R.L., Erickson, N.R., Dickman, R.L., Schloerb, F.P., and Irvine, W.M., Astrophys. J., in press.
7. "Astronomical Identification of the C_3H Radical", Thaddeus, P., Gottlieb, C.A., Hjalmarson, Å., Johansson, L.E.B., Irvine, W.M., Friberg, P., and Linke, R.A., Astrophys. J. Lett., submitted.

Future Plans

Large maps of ^{13}CO emission were made last year in three molecular clouds in the Taurus dark cloud complex and the L134N molecular cloud. The spatial

resolution of the FCRAO 14 m telescope on such nearby molecular clouds, which include sites of solar-type star formation, permits resolution of spatial scales as small as 0.03 pc (or 6000 AU). Along with other FCRAO colleagues, we have begun a more extensive mapping project to fully sample an even larger portion of this cloud complex. To date over 3600 additional spectra have been obtained; this study will continue through the following year, during which it is hoped that 4 square degrees will be fully mapped. The selection of most regions have been strongly biased toward chemically well studied areas, so that information on the physical and evolutionary state of these clouds will be available to our detailed chemical studies.

Isotopic fractionation can provide a sensitive probe of chemical processes in the interstellar medium. Observations of deuterium fractionation in HC_3N and HC_5N have strongly suggested that these species are produced by purely gas-phase processes. Unfortunately, corresponding data is not available for DCN/HCN , which is a possible parent of the longer molecules. We hope to obtain this data during the present observational season, in collaboration with our Swedish colleagues.

We plan a search at FCRAO for OCS in nearby cold, dark interstellar clouds in order to continue our study of sulfur-bearing compounds, the relative abundances of which will provide information on the possible role played by catalytic reactions on grain surfaces. Locations of peak emission from OCS will be used to guide a search for the heretofore undetected molecule OC_3S in interstellar clouds.

Searches will also be undertaken for new interstellar molecular species whose existence or lack thereof will provide constraints on models of interstellar chemistry. In particular, Ziurys will continue previous searches for protonated hydrogen cyanide (HCNH^+) and for NH_2 , and Ziurys and Irvine plan

a survey of molecular clouds for protonated carbon dioxide (HCO_2^+). The latter species, HCO_2^+ , has to date been detected only in the galactic center source SgrB2.

The abundance of C_2H plays an important role in chemical modeling of cold molecular clouds. Its value has been quite uncertain, however, because observations have been largely restricted to the strongest hyperfine component, which appears to be saturated. Friberg and Madden are planning to observe several of these components in molecular clouds in order to accurately determine abundances. In a related project, in collaboration with P. Thaddeus at Columbia University-NASA GISS, we plan a search for the deuterated counterpart, CCD. This species has recently been identified for the first time in the laboratory, and its rotational spectrum determined.

In collaboration with colleagues at the Nobeyama Radio Observatory in Japan, Friberg and Irvine plan to probe high density concentrations within the cold cloud TMCl by observing C^{34}S . By studying this rare isotopic species we can insure that problems of saturation are avoided (it seems quite likely that the common isotopic species does suffer from saturation and self absorption effects toward TMCl). Observations of the J=1-0 transition are planned at the Nobeyama Radio Observatory, and complementary observations of the J=2-1 line will be undertaken at the Onsala Space Observatory in Sweden. Since the diameters of these telescopes are in the ratio of 45/20 (Nobeyama/Onsala), while the frequencies of the transitions are in the ratio 2/1, the angular resolution obtained on the source will be almost equal in the two sets of observations, so that the results may be directly compared.

Study of the chemistry of extended stellar envelopes is important both as an aid to understanding the physical and chemical processes in these regions, and also because some of this molecular material may be incorporated into

surrounding molecular clouds. Ziurys plans a search for NO in oxygen-rich stellar envelopes. Some theoretical models of such envelopes predict that NO should be quite abundant.

A major, ongoing project is the study of chemical, physical, and kinematical conditions in the nearby cold clouds TMCl and L134N. Specifically, maps of both sources are being obtained in a number of molecular transitions over much more extensive regions in the cloud than have heretofore been sampled. This will provide a knowledge of the physical and dynamic state, which will then be used to interpret subsequent observations of additional molecular species at specific points of interest in the cloud. We believe such multi-spatial, multifrequency observations are essential in order to adequately understand the interlinked chemical and physical processes in interstellar clouds.

Personnel

Dr. P. Friberg from the Onsala Space Observatory in Sweden returned to the University of Massachusetts under a Post-Doctoral program supported by the Swedish Natural Sciences Research Council. Dr. Lucy Ziurys was hired in November, 1984, as a Post-Doctoral Research Associate at the FCRAO, supported half time by this grant.

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