Final Report

Chemical Constraints on the Early Solar System

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I. Statement of Research

Chemical abundances of comets and star-forming regions provide powerful clues to the conditions which prevailed in the outer solar nebula. Hence comparative spectroscopic studies of cometary and molecular cloud gases provide vital insights into conditions in the solar protoplanetary disk at heliocentric distances beyond 5 AU 4.6 Gyr ago. We proposed a research program which combined optical and sub-millimeter techniques with laboratory spectroscopy, and sought to determine key diagnostic constraints on single-star protoplanetary disk models.

II. Summary of Results

A. Molecular Abundances

Comet Hale-Bopp was discovered at a heliocentric distance of 7 AU, was monitored during its inner solar system trek, and is still being observed post-perihelion 12 AU from the sun. This was the first comet to show definitive evidence for reshuffling molecular abundances through coma chemistry (Irvine et al. 1998, Lovell et al. 1998, Rogers and Charnely 1998, Ziurys et al. 1999). In 1996 Comet Hyakutake provided a unique opportunity to observe a comet with unprecedented spatial resolution because of its close approach to the Earth ($\Delta < 0.1$ AU). X-ray radiation was detected in comets Hyakutake and Hale-Bopp, and attributed to an interaction between the expanding cometary plasma and the solar wind (Bingham et al. 1997, Häberlie et al. 1997, Cravens 1997, Owens et al. 1998).

We obtained both optical and mm wavelength spectra of the Oort cloud comet Hale-Bopp (C/1995 O1), and have analyzed near-simultaneous measurements of various transitions of HCN, HNC, CN and $HCNH^+$ (Ziurys et al. 1999). Three separate HCN transitions were observed, two of which had hf structure that could be partially resolved. Production rates, Q, were determined for parent species using a Monte Carlo coma model developed by us which balances sublimation rates from the comet nucleus with photodestruction rates to match the observed column densities. No such modeling was done for $HCNH^+$ because its origin was unlikely to be sublimation or photodestruction of a parent species. Production rate abundance ratios, Q/Q' derived for Hale-Bopp are summarized in Table 1 together with column density ratios N_{tot}/N'_{tot}, (Ziurys et al. 1999).

Table 1. Comet Hale-Bopp Abundance Ratios

Ratio	U. T. Date	N_{tot}/N'_{tot}	Q/Q'
HCN/HNC	3/7-3/9	7 ± 1	
$HCN/HCNH^+$	3/7-3/11	>1	
$HCN/H^{13}CN$	3/24-3/25	109 ± 22	100 ± 20
$HCN/HC^{15}N$	3/24-3/25	330 ● 98	286 ± 82
HCN/CN	3/7-3/8		3 ± 1
	3/24-3/25		3 ± 1

We found that the [HCN]/[CN] ratio in Hale-Bopp was ~3. Hence, HCN is sufficiently abundant to be the parent molecule of CN in Hale-Bopp, in contrast to what was found in other comets such as IRAS-Araki-Alcock (e.g. Bockelée-Morvan et. al. 1984). Our result is consistent with the suggestion that most of the cometary CN observed (with large field-of-view instruments) arises from grains rather than nucleus HCN ice (A'Hearn et al. 1995). We also found for Hale-Bopp that [HCN]/[HNC] ~7 near perihelion, indicative that HNC may have been produced by coma chemistry.

B. Isotopic Abundances

Carbon isotope abundance ratios provide important constraints on the formation environment of a comet. The bulk carbon isotope abundance ratio in the solar system determined for the sun, the outer planets is $^{12}C/^{13}C = 90$ (Anders and Grevesse 1989, Jaworski and Tatum 1991, Kleine, et al. 1995, Jewitt et al. 1997). This ratio represents the carbon isotope abundance present in the proto-solar nebula 4.6 Gyr ago when the solar system formed, since negligible isotopic fractionation has occurred since that time (Lécluse 1998). Recent analyses of carbon isotope ratios in comets indicate agreement with the solar system value for CN in comet Halley (Jaworski and Tatum 1991, Kleine, et al. 1995), and for HCN in comet Hale-Bopp (Jewitt et al. 1997, Ziurys et al. 1999).

We determined $^{12}C/^{13}C$ abundance ratios using a full fluorescence excitation model for comets Levy (C/1990 K1), Austin (C/1989 X1), and Okazaki-Levy-Rudenko (C/1989 XIX) (Wyckoff et al. 2000), and found carbon isotope ratios of 90±10, 85±20 and 93±20, respectively, consistent with the solar system ratio, 90. The lower limit for the nitrogen isotope ratio, $^{12}C^{14}N/^{12}C^{15}N \geq 200$, found for comet Levy is consistent with the solar system value, 272 (Wyckoff et al. 2000). Our mm wavelength spectra of HCN in comet Hale-Bopp were analyzed to derive carbon and nitrogen isotope ratios (Ziurys et al. 1999). Both values are close to the terrestrial ratios of $^{12}C/^{13}C = 89$ and $^{14}N/^{15}N = 270$ (e.g. Wilson and Rood 1994), and not the local interstellar ratios, which are $^{12}C/^{13}C \sim 77 \pm 7$ and $^{14}N/^{15}N \sim 450 \pm 22$. Our results are also in reasonable agreement with ratios obtained from the J=4→3 observations of HCN and its isotopomers by

Figure 1 -- Carbon isotope abundance ratios measured in 9 comets (Ziurys et al. 1999, Wyckoff et al. 2000).

The 14% difference found between the solar system (90) and the present solar neighborhood interstellar (ISM) $^{12}C/^{13}C$ ratio (77±7) (Wyckoff et al. 2000), may be indicative of significant

Galactic ^{13}C-enrichment which has occurred in the interstellar medium (ISM) over the past 4.6 Gyr. The carbon isotope ratio measured in the present-day interstellar medium (ISM) toward the galactic center is about 20, increasing to 53±4 at the 4 kpc molecular ring and to 77±7 at the solar system ring (8.5 kpc)(Wilson and Rood 1994). Consistency among the ISM carbon isotope abundance ratios determined from several molecular species, CH^+, CO, CN, HCN, indicates that these ratios are relatively well-determined and free from chemical fractionation effects (Crane et al. 1991, Hawkins et al. 1993, Wilson and Rood 1994).

The two stable isotopes of carbon (^{12}C and ^{13}C) have been produced over the history of the Galaxy by explosive and hydrostatic helium burning in massive, intermediate and low mass stars. Carbon enrichment of the Galactic interstellar medium (ISM) has occurred sporadically by supernovae, and continuously by red giant stellar winds. One Galactic chemical evolution model has been constructed which matches (within a factor of two) the solar system elemental and isotopic abundances from hydrogen to zinc (e.g. Timmes et al. 1995). This model indicates that the bulk of the solar system carbon (about two-thirds) was generated by Type II and Type Ia supernovae, and the remaining one-third of the solar system carbon can be attributed to low and intermediate mass asymptotic branch stars which have dredged up ^{13}C-enriched material and gradually expelled it into the ISM over the past 4.6 Gyr. (Timmes et al. 1995). Thus the ^{13}C enhancement in the solar system (90) compared to the local ISM (77) may be due largely to gradual mass loss by red giant stars over the past 4.6 Gyr.

However, the high solar metal abundance, Z=0.02 plus the large solar system carbon isotope ratio may indicate that the solar system abundances are not representative of the Galactic ISM at the solar ring (8.5 kpc) 4.6 Gyr ago (e.g. Trimble 1991, Wilson and Rood 1994, McAndrew 1997). In fact chemical inhomogeneities on scales smaller than star forming regions are indicated by: 1) variations in the metal abundances among stars within the Orion association and 2) the large dispersion in metal abundances among halo dwarfs (McAndrew 1997). Such inhomogeneities may need to be incorporated into Galactic chemical evolution models to account more accurately for both the solar system carbon isotope ratio and the solar metal abundance (Wyckoff et al. 2000).

To follow up on this interesting result, we observed CN in a sample of molecular clouds using millimeter-wave techniques to study the galactic $^{12}C/^{13}C$ Ratio as a function of time and space in the Galaxy (Savage et al. 2002). The $N = 1 \rightarrow 0$ transitions of ^{12}CN and ^{13}CN ($X^2\Sigma^+$) at 113.5 and 108.8 GHz, respectively, were observed in a sample of thirteen Galactic molecular clouds using the Kitt Peak 12-meter radio telescope. The objects studied included the Galactic center (SgrB2(OH)), sources in the solar neighborhood such as Orion A and NGC 2024, and various other clouds with and without star formation. Hyperfine structure, arising from the nitrogen nuclear spin, was resolved in the spectra of both species, enabling an accurate determination of the opacity in ^{12}CN. From these measurements, estimates of the $^{12}C/^{13}C$ isotope ratio were obtained for the objects observed; these values fell in the range $^{12}C/^{13}C \sim 20$-70 and exhibited a noticeable gradient with distance from the Galactic center. In general, the ratios obtained from CN were very similar to those determined from millimeter observations of CO, but were consistently lower than those derived from H_2CO. The $^{12}C/^{13}C$ ratio of 43 ± 7, found in Orion A, is similar to that determined from optical observations of CN towards a nearby source, ζ

Ophiuchi. The lower carbon isotope ratios may indicate some chemical fractionation in CN, which is formed independently of CO and has a comparable difference in zero-point energies for the ^{12}C and ^{13}C isotopomers. The highest ratios (65 ± 12 and 70 ± 11), were obtained towards two known PDR regions (Orion Bar and NGC 2024); CN in these two sources may be undergoing some isotope-selective photodissociation. This study (Savage et al. 2002) additionally suggests that millimeter transitions of CN can also be used as useful tracers of the $^{12}C/^{13}C$ ratio in the Galaxy.

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