An Analysis of How the Relative Amounts of Hydrogen Cyanide Vary as Comet Hale-Bopp Approaches the Sun

Maegan Rosenberg

Briarcliff High School

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Abstract

We measure the 88 GHz, 177 GHz and 265 GHz lines of hydrogen cyanide (HCN) in NRAO 12-m telescope spectra of Comet Hale-Bopp collected during the comet's 1997 apparition. The inferred column densities of HCN range from 8.26 x 10^9 to 3.32 x 10^{13} cm -2 and vary in a regular way correlated with the comet-Sun distance, and therefore the degree of solar irradiation. The spectral lines were extracted from raw spectra using the GILDAS/CLASS spectral analysis package. Line strengths were measured using the Gaussian line fit procedure, and strengths range from 0.2 to 1.5 K km/s. The results confirm our hypothesis that as Hale-Bopp approaches the Sun, the mass of HCN released by the comet increases. During October of 1996, the relative amounts of HCN released vary from 8.26 x 10^9 to 1.32 x 10^{11} , while during March of 1997, when Hale Bopp reached perihelion, meaning it was the closest distance to the Sun that it would be throughout its orbit, the results increased to 3.32 x 10^{13} , further confirming the hypothesis.

1.0 Review of Literature

It was long been known and accepted that comets mainly consist of ice, rock, dust, and frozen gas. In 2011, Paul Hartogh and his team found that water in the ice from Hartley 2/Comet 103P had a very similar D/H ratio to that of Earth's oceans. D/H ratio is the ratio of deuterium to hydrogen, and the water analyzed from Hartley 2 had a D/H ratio of (1.61 +/- 0.24) x 10^-4. This was a shocking finding, as the average D/H ratio from six comets that were studied in the past was found to be (2.96 +/- 0.25) x 10^-4. The mean D/H for ocean water on planet Earth is currently (1.558 +/- 0.001) x 10^-4;

which is very similar to the D/H ratio found in comet Hartley 2. A possible explanation for this is that the six comets that were previously analyzed all originated from the Oort Cloud, while Hartley 2 belongs to the JF (Jupiter Family) comets, which are believed to have originated from the Kuiper Belt. Either way, this is an interesting find and might suggest that comets brought ocean water to this planet, or at the very least, is intriguing, as it shows that two bodies of water, hundreds of astronomical units apart, can have the same D/H ratio.

As mentioned before, what makes comets so fascinating is that they consist mainly of frozen water, and theory suggest that comets may have been the ones to bring water to this planet, and that the frozen ice contains matter from the birth of the Solar System. Rotational spectroscopy, which measures the energy levels of transitions that occur between quantized rotating molecules in a gaseous phase, can be used to study the ice in comets without actually physically having the ice in person (Hartogh, et al 2009). In 2015, Decock and his team used the PACS, (Photodetector Array Camera and Spectrometer) of the Herschel Space Observatory, to study the rotational spectroscopy of water in Comet 10P/Tempel 2, 103P/Hartley 2, 45P/Honda-Mrkos-Pajdusakova, and C/2009 P1 (Garradd). This was an interesting choice of comets because it included comets from the Oort Cloud (45P, 10P, and P1) being studied with the same PACS as a JF comet (103P). The results showed that the flux intensity (Jy) of H_2O in Comet 103P was greater than 4 Jy, and present at the wavelengths 108, 114, 124, 133, 136, 138, and 145 μm. However, a different wavelength range (that of 140 to 180 μm) record on the same day, November 11th 2010, shows the flux intensity of H_2O being greater than 13 Jy, and being present at wavelengths 153, 170, 182, and 187 μm.

At both wavelength ranges, the flux intensity of OH remained low and below 1 Jy, but spiking at random intervals. Though this seems confusing, it is a good example of how rotational spectroscopy can be used to be analyze matter that is astronomical units away, and something I need to understand, as my project will be using rotational spectroscopy to obtain data. Rotational spectroscopy has been in used in many experiments involving planetary bodies since its usefulness was discovered. It detected ammonia in comet 67P (N. Biver et al, 2015), helped to calculate a synthetic spectrum Comet C/2001 A2 based on its collection of data on how hydrogen behaves at certain wavelengths (Feldman, 2015). H. Weaver used rotational spectroscopy in 2012 to determine the ultraviolet spectrum of the gases in Comet ISON. Though this may sound unremarkable, the point is that this method can obtain data from bodies that are astronomical units away, without having to spend billions of dollars on a space mission to physically interact with the comet.

Comets are considered to be the building blocks of the cores of planets, and understanding their chemistry and physical makeup could provide crucial information on how the Solar System was formed (A’Hearn, 2011). Photometric and spectroscopic surveys of more than 100 comets have enabled taxonomic groupings based on free radical species and on crystallinity of rocky grains. Comets can be grouped into taxonomic groupings which depend on the crystallinity of the rock grains that make up the cometary nucleus, and on the free radical species (Mumma & Charnley, 2011). The data to make these groupings is gathered from photometric and spectronic surveys. Nuclear spin ratio and isotopic ratios (such as D/H) are shown to impact the gas species in the comet’s nucleus, further diversifying comets from one another. As mentioned before, all comets are made of ice, rock, and dust, but what truly makes them different from one another is the frozen gas species that make up the comet's nucleus (Sandford, 2008). The most prominent gas that all comets seem to contain in their nuclei is carbon; the building block of life. Studying comets that were formed far from the Solar System would also show how the abundance of certain compounds differs from where the Solar System was formed, to other areas in the Universe. Sandford also believes that since comets contain organic compounds, that are believed to have been frozen in the comet's ice since the comet's origins, that comets could have played a role in bringing life to Earth.

This interesting theory about comets is that they brought DNA to Earth, or, in other words, brought life to this planet, the first step in a long path of evolution that brought humanity to where it is today (Lin, Loeb, 2015). The point of Lin and Loeb's research was to try and theorize whether or not it was possible for DNA to survive travel in space, as they were researching the origins of life on this planet, a long-asked, and even controversial question. By analyzing already known data on comets and the distances between key comets and Earth, they concluded that if life did come from anywhere besides Earth, they likely would have been brought here by comets, though it's still not sure whether or not life did start in another location. The paper also brings up the Fermi paradox (Adami, 2000), which asks if extraterrestrial beings exist and started evolving at the same point in time that Earth life did, then why haven't we heard from them yet? This is an interesting field of study, and a theory that makes comet research especially fascinating.

Atoms and molecules have discrete energy states as described by quantum mechanics. In the case of atoms, the energy states are determined by the interactions between the electron and nucleus. As the simplest example, the hydrogen atom has a set of allowed electron energy states (labelled with the quantum number n) shown below.

When an electron drops down in energy between two of these states, a photon is emitted with an energy corresponding to the difference in energy between the two states. For instance, a jump between n=3 and n=2 produces a photon with (-1.511 eV - (-3.4 eV))= 1.889 eV which corresponds to a wavelength of 656 nanometers, in the red part of the spectrum. Jumps between n=4 and n=2 produce a green photon, between n=5 and n=2 a blue photon, and so on. This is the distinctive visible spectrum of hydrogen atoms which allows us to identify the atom even in deep space

Molecules also emit photons, not because of electron-nucleus interactions but because of atom-atom interactions. The molecules can only rotate or vibrate at certain rates, and any change between one rotational state and another will produce a distinctive photon of a given frequency. The energy jumps that molecules undergo are much lower energy than for atoms, so the emitted photons are in the long-wavelength radio part of the electromagnetic spectrum. Since we can not see radio waves with our eyes, there is no corresponding picture of the spectrum, but radio receivers can detect them and we can plot the results.

Observations taken with the 12-m NRAO telescope can be tuned to particular radio frequencies to detect photons from particular molecules. For instance, the plots two different transitions of the molecule HCN (hydrogen cyanide) can be plotted.

The area under each curve is proportional to the number of photons of each frequency received at the telescope which is related to the total number of molecules evaporating from the comet. By comparing the number of photons we receive at each frequency, we can determine important properties like the temperature of the HCN molecules and the total number of molecules. We can then compare these at different points in the comet's orbit to see how the molecule formation rate depends on distance from the Sun.

2.0 Methods

The data was provided by Stefanie Milam, a solar systems' astronomer at NASA Goddard Space Flight Center. Data was collected by using radio recievers on the National Radio Astronomy Observatory 12-meter Telescope, located on Kitt Peak in Arizona. The 12-m was a workhorse of radio astronomy for solar system and interstellar science for nearly 50 years. For this project, the 12-m was used to measure the raw spectra of HCN. The raw spectra are then divided by atmospheric transmission in the relevant band to get calibrated spectra. Then, using the distance between the comet and the telescope, we can convert line intensities (power per area reaching the telescope) into production rates. The data was collected from October 1996 to June 1997, but HCN was only measured in October of 1996, March of 1997, May of 1997, and June of 1997. The data are spectra of molecules which give off radiation at wavelengths between 1mm and 4mm, corresponding to frequencies of 75-300 GHz. The first step was to find the velocity-integrated line intensity, $T_R \Delta V$, where T is the frequency-dependent antenna tempearture and V is the velocity of the emission. This was done using the program GILDAScite, which is a computer program designed toward analyzing submillimeter radio astronomical applications.

$T_R \Delta V$ was then put into the formula

$$n(\text{total}) = 3k\, T_R \Delta V_{1/2} \mathbf{5}\text{rot}/(8\boldsymbol{\pi}^3 v S_{ij} u^2{}_0 e^{-\Delta E/kTrot}),$$

where k=Boltzmann's constant, $T_R \Delta V$ equals the area of the HCN lines, **5**rot equals the rotational partition function, v equals the frequency of the transition, Sij is the transition line strength, μ is the dipole moment of the HCN molecule, and T_{rot} is the rotational temperature of the emission, assumed here to be 50 K. This equation then gives the column density of molecules (number per square centimeter) within the telescope beam.

To create each graph, a set of commands were input in to the GILDAS program

{ file in mar97.class/may97.class/oct96.class {Reads designated file into memory}

find {Finds observations}

set source HJAB/HAILJABBA/HALEBOPP {Sets the source of the observations}

find {Finds observations}

set frequency (insert frequency number) {Sets the frequency of the observations}

find {Finds observations}

set scan (insert scan number) {Sets number of observations}

find {Find observations}

average /nocheck /resample {Complies data into a format in which it can be plotted}

plot {Plots emission spectra}

set window (use cursor to draw window) {Sets window of plot} lines ½ (lines depends on how many peaks are present in the graph; boundaries of each lines are placed on boundaries of peak) {Lines are put at peak boundaries}

method gauss {Sets that data will be calculated using GAUSS method}

base 0 {Cuts off graph at x=0}

minimize {Compiles data → final step towards finding area underneath peaks}

visualize {Draws green line which shows line what area is being used in calculation}

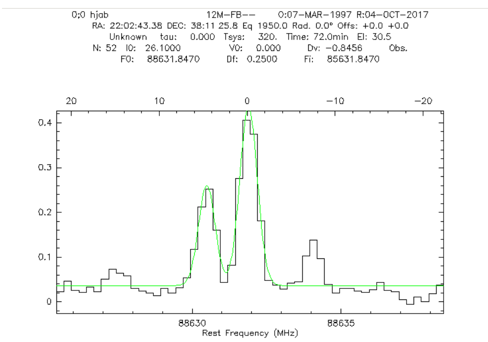
The result is a graph showing the intensity of HCN emission at the selected frequency as a function of velocity on the chosen observation date. This process is repeated for each frequency and observation date.

3.0 Results

3.1 Frequency 88631.8470

Figure 1

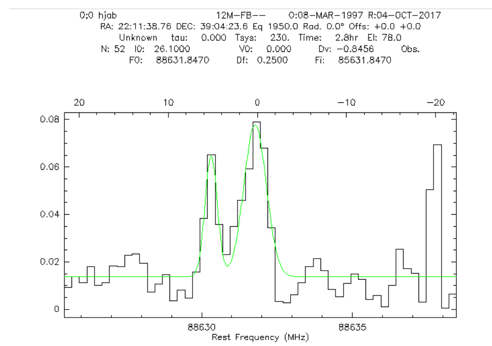
Line	Area		Position		Width		Tpeak
1	0.15516	(0.016)	-1.354	(0.034)	0.653	(0.076)	0.22330
2	0.29287	(0.017)	0.048	(0.020)	0.692	(0.043)	0.39751



Data taken on March 7th 1997, on the scan 1813-1815, with two peaks appearing at 0, and 5. There is a slight peak at -8 as well. The area underneath the first peak Is equal to .15516, while the second peak is equal to .29287

Figure 2

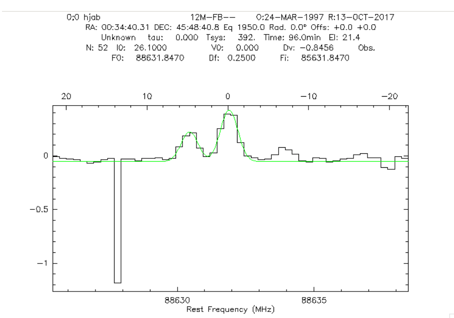
Line	Area		Position		Width		Tpeak
1	2.59372E-02	(0.007)	-1.531	(0.060)	0.479	(0.136)	5.09216E-02
2	5.93838E-02	(0.009)	-0.073	(0.069)	0.871	(0.144)	6.40628E-



Data taken on March 8th 1997, with two peaks appearing at 5 and 0. The spike at -20 can be inferred to be a system error. The area underneath the first peak at 0 is equal to 5.94 x 10^-2, while the area underneath the second peak, at 5, is equal to 2.59 x 10^-2

Figure 3

Line	Area		Position		Width		Tpeak
1	0.21134	(0.123)	-1.397	(0.222)	0.721	(0.489)	0.27555
2	0.38074	(0.115)	0.048	(0.110)	0.747	(0.263)	0.47875

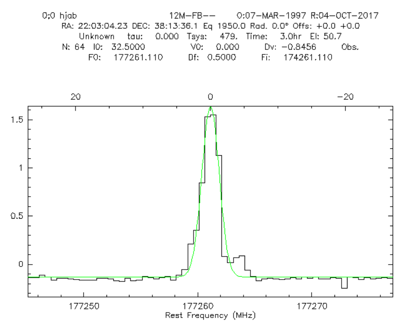


Data taken on March 24th 1997, on the scan 2603-2606. The first spike occurs at about 5, and the area recorded underneath is equal to .21134. The second spike occurs at 0, with the area underneath equal to .38704. The large dip recorded at 12 is likely due to a system error.

3.2 Frequency 177261.110

Figure 4

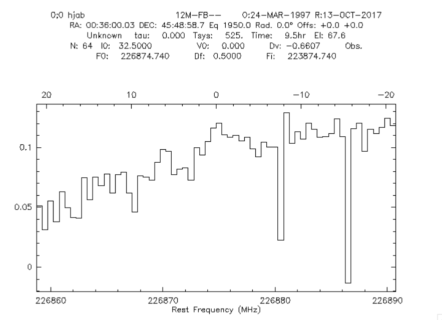
Line	Area	Position	Width	Tpeak
1	3.3637 (0.060)	0.012 (0.015)	1.788 (0.039)	1.7675



Data taken on March 7th 1997, on the scan 1819-1831. Here there is one peak at 0, and the area underneath the peak is equal to 3.3637.

Figure 5

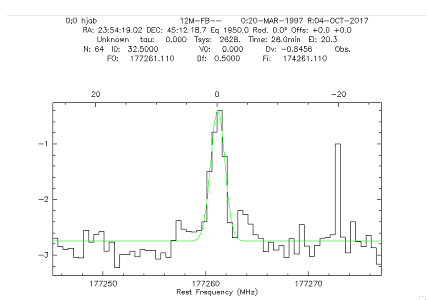
Line	Area	Position	Width	Tpeak
1	4.0446 (0.440)	0.068 (0.085)	1.618 (0.209)	2.348



Data taken on March 24th 1997, on the scan 2269-2274 This data may be inaccurate due to the large number of peaks on this particular scan. The highest peak is recorded at 0, and the area underneath this peak is equal to 4.0446

Figure 6

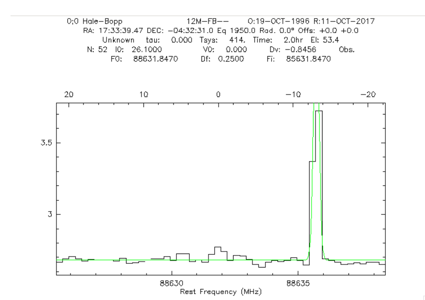
Line	Area	Position	Width	Tpeak
1	5.1921 (0.293)	-0.098 (0.053)	1.946 (0.136)	2.5065



Data taken on March 20th 1997. The peak appears at 0. The Second peak, which appears at -20, is believed to be another systems error

Figure 7

Line	Area	Position	Width	Tpeak
1	0.45725 (0.010)	3.869 (0.002)	0.250 (0.130)	1.7182

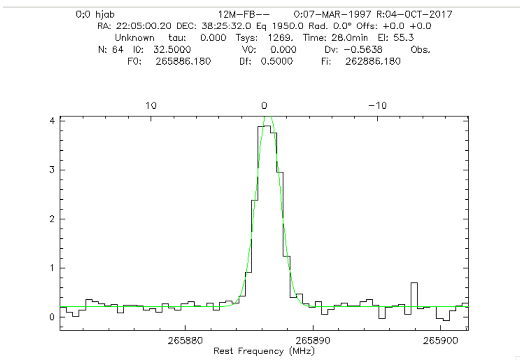


Data taken on October 19th 1996, on the scan 154-158. Though it appears that a peak occurs at -12, this is believed to have been another error. The errors appear to consistently appear around -15 to -20.

3.3 Frequency 265886.180

Figure 8

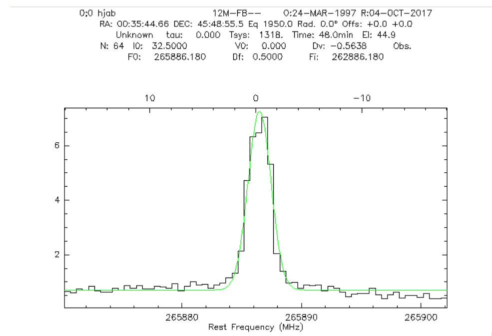
Line	Area		Position	Width	Tpeak
1	9.2345	(0.179)	0.309 (0.021)	2.147 (0.046)	4.0405



Data taken on March 7th 1997, on the scan 1866-1871, The peak appears at 0, which is consistent with data from the other frequencies The area under the peak is equal to 9.2345.

Figure 9

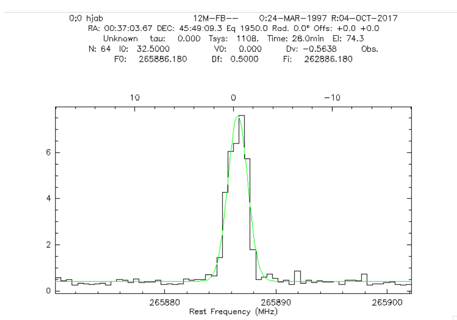
Line	Area		Position	Width	Tpeak
1	15.703	(0.263)	0.307 (0.018)	2.251 (0.043)	6.5522



Data taken on March 24th 1997, on the scan 2619-2620, with the peak appearing at 0. The area under the peak is equal to 15.703.

Figure 10

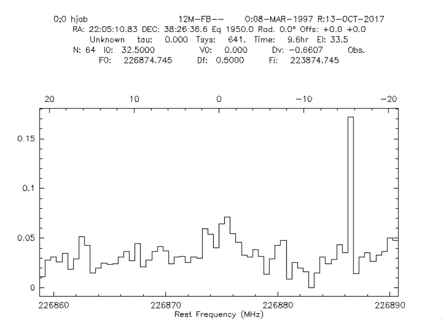
Line	Area		Position	Width	Tpeak
1	15.923	(0.188)	0.389 (0.012)	2.084 (0.027)	7.1768



Data taken on March 24th 1997, on the scan 2638-2639
The peak appears at -1, and the area underneath is equal to 15.923

Figure 11

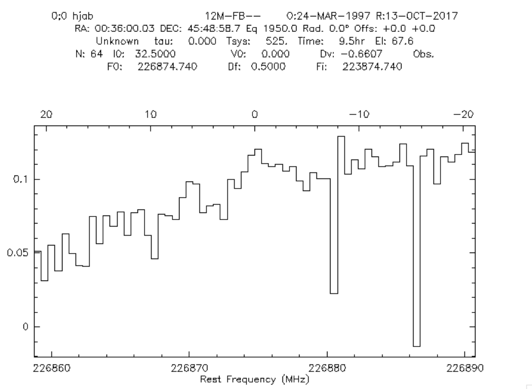
Line	Area	Position	Width	Tpeak
1	2.46467E-02 (0.017)	-1.033 (0.199)	0.522 (2.573)	4.43787E-02
2	5.99298E-02 (0.029)	0.700 (0.343)	1.432 (0.862)	3.93039E-0



Data taken on March 24th 1997, on the scan 1874-1897; the area underneath the lines represents the HCN emission on 3/24/97. There are two peaks, which appear around 0. The area underneath the two Peaks is equal to 2.46 x 10^-2 and 5.99 x 10^-2. The spike at -15 was Likely an error.

Figure 12

Line Area Position Width Tpeak
1 0.12763 (0.066) 1.128 (1.157) 4.211 (2.516) 2.84736E-02



Observations taken on March 24th 1997, on the scan 2621-2654. The data peak occurs at 0, and the area underneath this peak is equal to .12763. There are two dips at -8 and -15, believed to be a result of computing errors.

3.4 Molecule Rates

Figure 13

Mar-97	Date	Frequency	Scan	Lines	TRV (area)			Delta	R	dipole moment	k	Rotational Partition Function	Sij	e-Eu/kT	N_tot.	
done	3/7/97	88631.847	1813-1815	2	#1 = 15516, #2 = 29287			1.422 (6th)	1.026	2.98 Debye	1.38064x10^-16 cm2 g s	3.343	0.5555	0.085	9x10^10	
done	3/8/97	88631.847	1949-1955	2	593.86394			1.422 (6th)	1.026	2.98 Debye		3.343	0.5555	0.085	8.262E+09	
done	3/24/17	88631.847	2603-2606	2	#1 = 21134, #2 = 38704			1.316	0.926	2.98 Debye		3.343	0.5555	0.085	8.324907523 x 10^11	
done	3/7/97	1.7726111*	1819-1831	1	336370		bad fit	1.422	1.026	2.98 Debye		3.343	0.2500.	0.2552	6.076474819 x 10^12	
done	3/20/97	177261.11	2269-2274	1	404460			1.318	0.94	2.98 Debye		3.343	0.2500.	0.2552	7.3065107 x 10^11	
done		177261.11	2610-2614	1	519210					2.98 Debye		3.343	0.2500.	0.2552	9.379452649 x 10^11	
done	3/7/97	2.6588618*	1866-1871	1	923450		bad fit	1.422	1.026	2.98 Debye		3.343	0.2000.	0.5104	1.818517475 x 10^13	
done	3/24/97	265886.18	2638-2639	1	1592300		bad fit	1.316	0.926	2.98 Debye		3.343	0.2000.	0.5104	3.3162871023 x 10^13	
done	3/24/97	265886.18	2619-2620	1	1570300		bad fit	1.316	0.926	2.98 Debye		3.343	0.2000.	0.5104	3.092336337 x 10^13	
																;
Oct-96	10/19/96	88631.847	154-158	1	2240.34			3.040 (17)		2.98 Debye	1.38E-23	3.343	0.5555	0.085	3.141106005 x 10^10	
	10/20/96	88631.847	161-172	2	23093.58X			3.049 (22)		2.98 Debye	1.38E-23	3.343	0.5555	0.085	3.237837331 x 10^11	
	10/20/96	88631.847	177-192	2	#1 = -4.26326E-10, #2 = -1.59980E-10					2.98 Debye	1.38E-23	3.343	0.5555	0.085	x	
done	10/23/96	88631.847	428-433	2	8718.82			3.049		2.98 Debye	1.38E-23	3.343	0.5555	0.085	11958.086	
done	10/24/96	88631.847	558-562	2	9682.57					2.98 Debye	1.38E-23	3.343	0.5555	0.085	1.32798122 x 10^11	
done	10/25/96	88631.847	618-625	2	#1 = 2.68215E-02, #2 = 4.66173E-02			3.053 (27)		2.98 Debye	1.38E-23	3.343	0.5555	0.085	1.007225837 x 10^11	
done	10/25/96	88631.847	672-675	2	#1 = 3.71231E-02, #2 = 5.78346E-02					2.98 Debye	1.38E-23	3.343	0.5555	0.085	1.302361274 x 10^11	

On the table above, scan is equal to the observation number, lines is equal to how many peaks were shown in the molecular frequency graph, the area is equal to the area underneath the lines in the molecular frequency graphs, delta is equal to the comet's distance from the Sun, R is equal to the comet's distance from Earth, n_tot equals the number of molecules, and Sij is equal to spectroscopic values for hyperfine components of the lowest 5 downward J-level transitions.

4.0 Discussion

The results show that as Comet Hale-Bopp approaches the Sun, the measured amounts of HCN increase. The data was taken from two time periods, October of 1996, and March of 1997. Comet Hale-Bopp reached perihelion in March of 1997, where it was .914 AU from the Sun. During October of 1996, the Comet was approximately 3.05 AU from the Sun, and the measured amounts of HCN are much lower than they are in March of 1997. In October of 1996, the comet was approaching the Sun, while in March of 1997, the comet was the closest it would ever be to the Sun. October of 1996 is when the comet was first close enough for the molecular wavelengths to be observed from Earth.

The greatest molecular abundances occurred when the comet was closest to the Sun, on March 24th of 1997. On this date, the comet was the closest to the Sun that it would ever be, or in other words, when it reached perihelion. The high amounts of molecular abundancies (10^13 compared to 10^11/96 and other dates) supports the hypothesis that as the comet comes closer to the Sun, more cometary ice containing HCN is released into the gas phase.

It is important to point out that there are apparent sources of error in the dataset; there should be no spikes or peaks that occur around -20 and -15. These fluctuations can be attributed to atmospheric influence, or in other words, data from a source other than the comet, which was picked up the Arizona State Observatory.

5.0 Limitations

Some limitations of this study include the fact that the data is from 1996/1997, making it over 20 years old. The data needed to be this old because only in these years was Comet Hale-Bopp close enough to the Earth for the molecular abundancies of molecules to be recorded. Another limitation was the fact that this study was supposed to include other molecules besides HCN, but the data file that detailed the frequencies for other molecules was corrupted in the years that it has been stored on a computer. One last limitation was that one of the files had incorrectly been given the wrong date, and that data set remains missing.

6.0 Conclusions

The conclusions which can be drawn from this experiment are that as Comet Hale-Bopp approaches the Sun, the relative amounts of hydrogen cyanide increase. This is believed to be because as the comet nears the Sun, the comet enters a period of sublimation. Sublimation is the process by which an ice changes phase to gas without going through a liquid phase, and only occurs when the gas pressure is low enough, as will happen in space. (CO_2 – “dry ice” - is the classic example of sublimation) . Once the ice begins to sublimate, the gases are free to react with one another (although HCN is probably already in existence as one of the ice constituents – it probably doesn’t need to react with anything else for us to measure it). Thus, the molecular abundances increase. The data supports the hypothesis that as the comet approaches the Sun, more HCN is released into the gas phase. Future research could possibly include researching how the relative amounts of other molecules, for example methanol and formaldehyde, vary as Comet Hale-Bop approaches the Sun. The data set that was obtained from Stefanie Milam could still be further analyzed, as it contains data about other molecular transmissions.

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