Carbon Isotope Chemistry in Molecular Clouds

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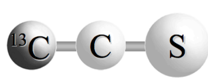
ABSTRACT

Few details of carbon isotope chemistry are known, especially the chemical processes that occur in astronomical environments like molecular clouds. Observational evidence shows that the $^{12}C/^{13}C$ abundance ratios vary due to the location of the ^{13}C atom within the molecular structure. The different abundances are a result of the diverse formation pathways that can occur. Modeling can be used to explore the production pathways of carbon molecules in an effort to understand and explain the chemical evolution of molecular clouds.

BACKGROUND

Isotopes are elements that share the same number of protons, but differ by the number of neutrons in the nucleus. When isotopes are found in molecular structures, the molecules are called isotopolouges, meaning at least one of the atoms is an isotope. An example is shown below:
Isotopolouges of the CCS molecule[6]



^{13}CCS

$C^{13}CS$

Observations have found an abundance difference between the two isotopic species, demonstrated by the abundance ratios below:[2]

(1) $[CCS]/[C^{13}CS] = 54\pm5$
(2) $[CCS]/[^{13}CCS\ ] = 230\pm130$
(3) $[C^{13}CS]/[^{13}CCS] = 4.2\pm2.3$

The inequality of the ratio values supports the theory that the abundances of the isotopolouges vary due to the location of the ^{13}C atom within the molecular structure. The differences of abundances are thought to be a result of different formation pathways.[3]

The abundance anomaly of the isotopolouges has been found in several molecular clouds, such as TMC-1 and L1521E, which suggests that dilution isn't unique to one enviroment.[3] The study of isotopolouges and their abundances are an important tool for understanding chemical processes in molecular clouds and other astronomical environments, such as protoplanetary disks.[3] Protoplanetary disk chemistry is of interest because the molecules that are formed and processed in the disk may later be incorporated into planetary material.[5]

PROGRESS

My work this summer has largely consisted of updating and revamping the current reaction sets in our molecular cloud model by adding the isotopolouges of the carbon species. Through a series of changing parameters in the code and graphing the abundances, the model began to coincide with the observational values. The results can be found in Table 1.

I also explored the importance of separating the branching ratios statistically and non-statistically. Branching ratios are the probabilities of reactants making certain products. Some products are more probable then others due to a variety of reasons. Some examples involve unpaired electrons, which makes the atom more reactive then other atoms that have a full valence shell. The structure of the molecule can also influence the outcome of the reaction depending on if the structure is linear or if it branches out.

RESULTS AND DISCUSSION

Table 1
Table of Abundances

Abundance Ratio	Literature Values from TMC-1	Our Values at 10^4 years	Our Values at 10^5 years	Our Values at $3x10^5$ years
CCH/^{13}CCH	>250 [2]	193	197	204
CCH/C^{13}CH	>170 [2]	111	121	91.8
C13CH/^{13}CCH	1.6 +/- 4 [2]	1.73	1.63	2.22
CCS/^{13}CCS	230 +/- 130 [6]	582	486	413
CCS/C^{13}CS	54 +/- 5 [6]	104	88.2	75.6
C13CS/^{13}CCS	4.2 +/- 2.3 [6]	5.62	5.51	5.47
CCCS/^{13}CCCS	>160 [6]	234	217	148
CCCS/C^{13}CCS	~ 60 [6]	221	136	124
CCCS/CC^{13}CS	~ 70 [6]	130	142	124
CCCCH/^{13}CCCCH	150 [6]	140	124	99.6
CCCCH/C^{13}CCCH	100 [6]	182	173	122
CCCCH/CC^{13}CCH	90 [6]	400	284	416
CCCCH/CCC^{13}CH	140 [6]	102	97.2	58.4

The values produced by our model do not match up precisely with the observations. This is to be expected because molecular clouds are remarkably complex systems and our model is only a simplified version. We will continue to add complexity to our model as we continue to make progress on the accuracy of the current model.

We also found that there was little difference between the statistical and non-statistical branching ratios. So for future models and studies we will save time by simply breaking up the probabilities statistically.

FUTURE WORK

We will continue fine-tuning the model in an effort to achieve better accuracy. We will consistently reference other observational values as a guide and other molecular cloud models as well.

Our model, though progressing, is not complete. One of the things we intend to study are the details of this reaction:

$^{13}C^{12}CS + S \Leftrightarrow {}^{12}C^{13}CS + S$

Understanding how this reaction occurs will add depth and accuracy to our model, which will then further our knowledge of interstellar chemistry. Does the $^{12}C^{13}CS$ form by the sulfur (S) simply tacking on to the end of the 13C atom? Or does the molecule break apart fully and then recombine? Answering these questions will be the next step for understanding chemistry other astronomical environments.

Another aspect of the model that will be explored is the sticking coefficient. The sticking coefficient models grain chemistry that happens in the molecular clouds. Grain chemistry is the interaction of the gaseous material and the solid grains found in molecular clouds. The molecules in the gas phase can react with the molecules that are frozen onto the surface of the grains. This can result in the molecules in the gas phase "freezing out" of the gas and onto the grains. The actual chemical rates of these processes are unknown. Currently, our model assumes that 30 percent of the gas molecules that interact with a grain will stick to it. Other models[1] have 100 percent of the gas molecules sticking when they encounter a grain. These parameters influence the time it takes for a cloud to evolve in the model and whether the freeze out of the molecules occurs at an earlier time, such as 10^4 years, or later, around 10^5 years.

This current model was compiled with the temperature set to 10K. In future models we will increase the temperature to 20K to see how that changes the chemistry in the molecular clouds. We anticipate seeing more CO chemistry in the clouds at this temperature because at 10K CO is frozen out of the gas phase.

Ultimately, we will expand our study to longer carbon chains, such as HC_5N, and publish our results.

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