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Chemical Simulations of Cyanomethanimine in Interstellar Medium

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Chemical Simulations of Cyanomethanimine in Interstellar Medium

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Abstract

Cyanomethanimine was recently detected in Sagittarius B2, an interstellar cloud known for its rich chemistry. Cyanomethanimine is a proposed intermediate in the interstellar synthesis of adenine. Adenine is crucial in the formation and maintenance of living systems due to its role as a major component in DNA/RNA. Unfortunately, it is not currently possible to obtain tangible chemical samples from Sagittarius B2, the interstellar cloud where cyanomethanimine resides, because it is too distant from the Earth. Furthermore, the best method for studying interstellar molecules for now is computer modelling. The objective of the project is to determine the abundance of cyanomethanimine in Sagittarius B2 through the utilization of computer modelling. The computer simulation uses a reaction network, several controlled parameters, and large differential equations to calculate the fractional abundances of molecules relative to hydrogen. Once the simulation was conducted, it was found that the peak fractional abundance of cyanomethanimine in Sagittarius B2 is 1.28×10^{-13}. More simulations will be needed to elucidate interstellar cyanomethanimine's behavior in regard to varying temperatures and densities.

Keywords/Phrases: Cyanomethanimine, Interstellar Medium, Astrochemistry, Adenine, Sagittarius B2

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Introduction

According to recent estimates, the observable Universe is approximately 90 billion light-years across (Halpern and Tomasello, 2016). Within the vastness of the Universe is predominantly empty space. However, a significant amount of matter is concentrated in regions such as stars, molecular clouds, and planets. Matter is manipulated in these areas over time through the star cycle. Stars are important factors in the formation of the elements that constitute chemical compounds. Stars can form elements from hydrogen to iron through nuclear fusion, a process which gives a star energy by smashing atoms together. Once a star begins to lose energy from nuclear fusion, it has a chance of exploding and spreading its contents across a region of space to form an atomic interstellar cloud. The atoms of the atomic interstellar cloud react over time to form a multitude of molecules, forming a molecular interstellar cloud. The molecular cloud can collapse once it reaches a high enough density. When the molecular cloud collapses, it can become a star-forming region due to increasing temperatures from the kinetic energy of the collapse (Kornreich, 2015). Eventually, stars are formed and the cycle continues.

Molecules from interstellar clouds can travel to planets and other regions of space via mobile rocky bodies such as asteroids or comets (Ehrenfreund and Cami, 2010). Molecules have a chance of reaching planets, which could expose the molecules to much different conditions than an interstellar cloud (Higher temperature, higher pressure, presence of an atmosphere, etc.). Consequentially, molecules could become more complex in structure, possibly even forming biological macromolecules like RNA (ribonucleic acid) or proteins. For example, the RNA world hypothesis asserts that the

origin of life on Earth began with the formation of RNA (Neveu et al., 2013). It is likely that primordial RNA formed from constituents originating from molecular clouds.

RNA consists of a repeating pentose sugar and phosphate backbone with four possible nitrogenous bases arranged along the backbone (Berg et al., 2015). Potential precursors of these nitrogenous bases have been detected in Sagittarius B2, a molecular cloud that is approximately 150 light years across (Chown, 1999). More specifically, a nitro organic molecule named cyanomethanimine (Figure 1) was detected in Sagittarius B2 by comparing spectra obtained from the Green Banks Telescope in West Virginia to experimentally-obtained spectra from the utilization of an electric discharge on gas phase acetonitrile and ammonia (Zaleski et al., 2013).

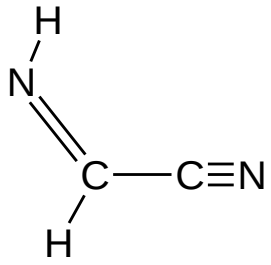

Figure 1. The structural formula for cyanomethanimine (HNCHCN), the prebiotic molecule of interest.

Cyanomethanimine is theorized to be a precursor to adenine (Figure 2), a purine base found in DNA and RNA (Roy et al., 2013). DNA and RNA are both essential for the existence of life because they store the biological information that allows an organism to develop and function. In the human body, two pathways exist for the synthesis of adenine

(and other nucleotides): The de novo pathway and the salvage pathway (Berg et al., 2015). Both pathways are proficient at creating nitrogenous bases required for DNA/RNA synthesis, but they both require enzymes in order to occur. Enzymes are typically large proteins consisting of many amino acid units. Enzymes are more than likely not found in interstellar medium due to their highly complex structure. As a result, the de novo pathway and salvage pathway found in most organisms cannot occur in interstellar medium. Instead, the synthesis of adenine in interstellar medium is thought to occur by way of hydrogen cyanide units (Roy et al., 2013). For example, adenine can be considered a hydrogen cyanide pentamer, which means that adenine consists of five hydrogen cyanide molecules. Cyanomethanimine is a dimer of hydrogen cyanide and is only the second proposed step in the interstellar adenine pathway.

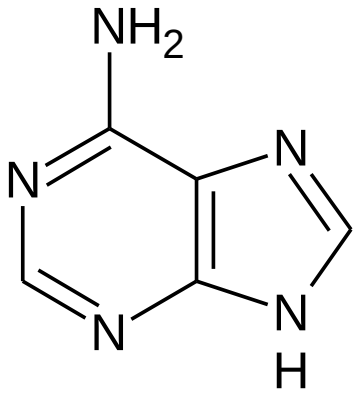

Figure 2. The structure of adenine, an important component of RNA and DNA (Berg et al., 2015).

Ultimately, the objective is to determine the abundance of cyanomethanimine in Sagittarius B2. A spacecraft armed with a mass spectrometer simply cannot be sent in a timely manner to Sagittarius B2 due to the limitations of current space propulsion technologies. While technology is advancing at an incredible rate, it will not likely be possible to analyze tangible chemical samples from Sagittarius B2 for many more decades.

Currently, computer modelling is the best method of determining chemical abundances in systems outside of the solar system. Using a computer allows for the simulation of Sagittarius B2 through the input of mathematical parameters that model similar conditions present in the interstellar cloud. The simulation includes a multitude of these parameters, the most important of which are temperature and density. A separate file from the parameters exists that contains a reaction/species network encompassing thousands of reactions found in Sagittarius B2 as well as a list of hundreds of species found in these reactions. The species are assigned charges and the number of each type of atom each species contains. Every reaction contains a unique set of α, β, and γ values that dictates the value of its rate constant. The Arrhenius equation (Figure 3) is the mathematical relation that determines the rate constant of a reaction and it is modified as an explicit function of temperature to give the α, β, and γ values (Figure 4). Also, every reaction is assigned a number (0-13 for gas phase reactions) that corresponds to a reaction type. Each rate constant for every reaction is ultimately incorporated into the differential equation that determines abundances of the compounds in the network to be multiplied in each of their respective terms.

$$k = A\, e^{-Ea / RT}$$

Figure 3. The Arrhenius equation models the rate of a reaction. The rate constant is k, A is the pre-exponential factor, e is an irrational constant, E_a is the activation energy, R is the universal gas constant, and T is temperature (Engel and Reid, 2014).

$$k(T) = \alpha\,(T/300)^{\beta}\,e^{-\gamma/T}$$

Figure 4. The Arrhenius equation is modified as an explicit function of temperature. The rate constant is k(T), α is the equivalent of a pre-exponential factor, T is the temperature, β is a pure number, e is an irrational constant, and γ is considered an activation energy.

Methods

The project began with an extensive literature search in order to learn the basics of astrochemistry. Eric Herbst's "The Chemistry of Interstellar Space" served as an invaluable learning tool for learning about the physical conditions in interstellar medium, the methods astronomers employ to study molecular clouds, the differential rate equation, the importance of dust grains, and the different types of reactions that occur in interstellar environments. Another important journal article detailed the detection of E-cyanomethanimine in interstellar medium through the comparison of experimental spectra with survey spectra (Zaleski et al., 2013). Along with its discussion of the detection of cyanomethanimine, the article discusses energetic considerations of the isomers (E, Z, and N). The Z isomer is the most stable, so the α, β, and γ values for the Z-isomer were used in the reaction between CN and CH_2NH that forms cyanomethanimine

(Vazart et al., 2015). The most stable isomer will likely have the greatest abundance. First and foremost, the goal is to determine if cyanomethanimine can form in significant amounts at all in interstellar medium. If the α, β, and γ values of the least stable isomer were used, the fractional abundance could possibly be much lower. While only the Z-isomer was considered, future work will likely involve all three isomers.

New gas phase reactions gathered from online astrochemical databases were added to the already existing reaction network, which initially contained 6597 reactions. By the end of the project, the network reached 6816 reactions and the list of species also increased from 689 species to 718 species (listed in Table 1). The majority of the new reactions were ion-molecule reactions, charge exchange reactions, neutral-neutral reactions, and dissociative recombination reactions. A few redundant reactions were added mistakenly ($\alpha = 0$), but they were left in the network because they do not impact the simulations at all. New grain reactions were not added. When adding the reactions to the network, reactant species were placed on the left and the products on the right, followed by the α, β, and γ values, the reaction type number, number of reaction in the reaction category, and the total number of reactions. Some reactions were developed that were not found in a database, but were necessary to bridge the gap between already existing molecules in the network to cyanomethanimine. As a solution, the α, β, and γ values were obtained from similar reactions for the bridging reactions. Once a sufficient number of reactions bridging cyanomethanimine to other species were added, any duplicate reactions found in the network were deleted.

After the reaction network was complete, the important files for the chemical simulations were studied to obtain a better understanding of how the computations are

conducted. Afterward, the density and temperature parameters in the control file were adjusted to 2 x 10^4 cm^{-3} and 10 K, respectively. After some troubleshooting involving reaction number errors, the simulation was conducted.

SPECIES	CHARGE	H	HE	C	N	O	S
H2CCN	0	2	0	2	1	0	0
CCN	0	0	0	2	1	0	0
HC2N	0	1	0	2	1	0	0
CH3OCH2	0	5	0	2	0	1	0
CH3O	0	3	0	1	0	1	0
HNCSH+	1	2	0	1	1	0	1
H2NCS+	1	2	0	1	1	0	1
NCCN+	1	0	0	2	2	0	0
CH3CNH+	1	4	0	2	1	0	0
HNCS	0	1	0	1	1	0	1
HNCHCN	0	2	0	2	2	0	0
NCSH	0	1	0	1	1	0	1
CCH	0	1	0	2	0	0	0
HC2N+	1	1	0	2	1	0	0
CSH+	1	1	0	1	0	0	1
HSCN	0	1	0	1	1	0	1
HCNSH+	1	2	0	1	1	0	1
HCNH+	1	2	0	1	1	0	0
H2SCN+	1	2	0	1	1	0	1
HNCS+	1	1	0	1	1	0	1
NCSH+	1	1	0	1	1	0	1
CCS	0	0	0	2	0	0	1
HCNS	0	1	0	1	1	0	1
NCHCN	0	1	0	2	2	0	0
HNCCN	0	1	0	2	2	0	0
NCCN	0	0	0	2	2	0	0
HNCHCN+	1	2	0	2	2	0	0
NCHCN+	1	1	0	2	2	0	0
HNCCN+	1	1	0	2	2	0	0

Table 1. A table listing the species added to the network, along with charges and the number of each type of atom (McElroy et al., 2012; Wakelam et al., 2017; Manion et al., 2015).

Reactions						α	β	γ
C+	H2CCN	C	CH2CN+			1.00E+00	1.61E-09	5.81E+00
HCS+	NH2	H	H2NCS+			9.88E-01	8.99E-10	4.69E+00
HCS+	NH2	H	HNCSH+			1.83E-03	8.99E-10	4.69E+00
H3O+	HNCS	H2O	HNCSH+			5.00E-01	1.54E-09	2.92E+00
H3O+	HNCS	H2O	H2NCS+			5.00E-01	1.54E-09	2.92E+00
H3+	HNCS	H2	HNCSH+			5.00E-01	3.47E-09	2.92E+00
H3+	HNCS	H2	H2NCS+			5.00E-01	3.47E-09	2.92E+00
HNCS	N2H+	N2	HNCSH+			5.00E-01	1.33E-09	2.92E+00
HNCS	N2H+	N2	H2NCS+			5.00E-01	1.33E-09	2.92E+00
H3O+	NCSH	H2O	HNCSH+			1.00E+00	1.43E-09	5.17E+00
C+	CCN	C	CNC+			4.00E-01	1.30E-09	6.20E-01
C+	CCN	CN	C2+			3.00E-01	1.30E-09	6.20E-01
CCN	HCO+	CO	HC2N+			1.00E+00	1.19E-09	6.20E-01
C+	CCN	C	C2N+			3.00E-01	0.00E+00	0.00E+00
H3+	NCSH	H2	HNCSH+			1.00E+00	3.20E-09	5.17E+00
N2H+	NCSH	N2	HNCSH+			1.00E+00	1.23E-09	5.17E+00
CSH+	NH2	H	H2NCS+			8.39E-01	8.99E-10	4.69E+00
CSH+	NH2	H	HCNSH+			1.54E-01	8.99E-10	4.69E+00
CSH+	NH2	CS	NH3+			1.36E-03	8.99E-10	4.69E+00
CSH+	NH2	NH2	HCS+			6.25E-03	8.99E-10	4.69E+00
CSH+	NH3	H2	H2NCS+			3.42E-01	9.51E-10	3.77E+00
CSH+	NH3	H2	HNCSH+			9.60E-07	9.51E-10	3.77E+00
CSH+	NH3	CS	NH4+			5.70E-01	9.51E-10	3.77E+00
CSH+	NH3	NH3	HCS+			8.79E-02	9.51E-10	3.77E+00
HNC	H2S+	H	HNCSH+			1.00E-01	9.97E-10	6.41E+00
HNC	H2S+	HS	HCNH+			9.00E-01	9.97E-10	6.41E+00
H3+	HSCN	H2	H2SCN+			5.00E-01	3.20E-09	5.17E+00
H3+	HSCN	H2	HNCSH+			5.00E-01	3.20E-09	5.17E+00
HCO+	HNCS	CO	H2NCS+			5.00E-01	1.32E-09	2.92E+00
HCO+	HNCS	CO	HNCSH+			5.00E-01	1.32E-09	2.92E+00
HCO+	HSCN	CO	HNCSH+			1.00E+00	1.18E-09	5.17E+00
CS	NH3+	H	H2NCS+			1.00E-09	-4.00E-01	0.00E+00
CS	NH2+	H2NCS+				2.40E-11	-1.00E+00	0.00E+00
HE+	HNCS	HE	HNC	S+		3.00E-01	3.00E-09	2.92E+00
HE+	HNCS	HE	HCN	S+		2.00E-01	3.00E-09	2.92E+00
HE+	HNCS	H	HE	CN	S+	3.00E-01	3.00E-09	2.92E+00

HE+	HNCS	HE	CS	NH+		1.00E-01	3.00E-09	2.92E+00
H+	HNCS	HNC	HS+			3.00E-01	5.90E-09	2.92E+00
H+	HNCS	NH	HCS+			2.00E-01	5.90E-09	2.92E+00
C+	HNCS	CS	HNC+			8.00E-01	1.85E-09	2.92E+00
C+	HNCS	C	HNCS+			1.00E+00	1.85E-09	2.92E+00
HNCS	HE+	HE	HNCS+			1.00E+00	3.03E-09	2.92E+00
H+	HNCS	H	HNCS+			1.00E+00	5.91E-09	2.92E+00
HNCS	S+	S	HNCS+			1.00E+00	1.29E-09	2.92E+00
H+	NCSH	H	NCSH+			1.00E+00	5.46E-09	5.17E+00
HE+	NCSH	HE	NCSH+			1.00E+00	2.80E-09	5.17E+00
HCCN	H+	H	HC2N+			0.00E+00	0.00E+00	0.00E+00
CH3+	HNC	CH3CNH+				9.00E-09	-5.00E-01	0.00E+00
CH3+	HCN	CH3CNH+				9.00E-09	-5.00E-01	0.00E+00
C2	CH+	H	C3+			5.00E-10	0.00E+00	0.00E+00
C2	CH+	CCH	C+			2.70E-10	0.00E+00	0.00E+00
C2	CH+	C	C2H+			1.80E-10	0.00E+00	0.00E+00
C2	CH+	C3	H+			5.00E-11	0.00E+00	0.00E+00
CS	HCO+	CO	HCS+			1.00E+00	1.16E-09	3.28E+00
CS	HCO+	CO	CSH+			3.00E-08	1.16E-09	3.28E+00
CS	H3+	H2	HCS+			9.65E-01	2.85E-09	3.34E+00
CS	H3+	H2	CSH+			3.50E-02	2.85E-09	3.34E+00
CS	H3O+	H2O	HCS+			1.00E+00	1.33E-09	3.28E+00
CS	H3O+	H2O	CSH+			3.15E-08	1.34E-09	3.34E+00
CS	HCNH+	HCN	HCS+			1.00E+00	1.20E-09	3.28E+00
HNCHCN	H+	NCHCN+	H2			6.00E-10	-5.00E-01	0.00E+00
HNCHCN	H+	HNCCN+	H2			7.50E-09	-5.00E-01	0.00E+00
HNCCN	H+	HNCCN+	H			4.00E-09	-5.00E-01	0.00E+00
HNCCN	H+	NCCN+	H2			6.00E-10	-5.00E-01	0.00E+00
NCCN	HE+	CN	CN+	HE		2.70E-09	0.00E+00	0.00E+00
NCHCN	H+	NCCN+	H2			7.50E-09	-5.00E-01	0.00E+00
HNCCN+	C2H4	C2H5+	NCCN			5.60E-10	0.00E+00	0.00E+00
C2H2	C2N2+	C2H2+	NCCN			5.80E-10	0.00E+00	0.00E+00
HNCCN+	CH3OH	CH3OH2+	NCCN			1.50E-09	-5.00E-01	0.00E+00
C2H4	C2N2+	C2H4+	NCCN			1.30E-09	0.00E+00	0.00E+00
H2O	HNCCN+	H3O+	NCCN			5.10E-10	-5.00E-01	0.00E+00
HCN	HNCCN+	HCNH+	NCCN			2.00E-09	-5.00E-01	0.00E+00
NH3	HNCCN+	NH4+	NCCN			2.00E-09	-5.00E-01	0.00E+00
HCN	C2N2+	HCN+	NCCN			5.40E-10	-5.00E-01	0.00E+00
C+	NCCN	C2N+	CN			2.00E-10	0.00E+00	0.00E+00

C+	NCCN	CNC+	CN			1.70E-09	0.00E+00	0.00E+00
C2H3+	NCCN	HNCCN+	C2H2			1.10E-09	0.00E+00	0.00E+00
H3+	NCCN	HNCCN+	H2			2.80E-09	0.00E+00	0.00E+00
HCO+	NCCN	HNCCN+	CO			1.30E-09	0.00E+00	0.00E+00
N+	NCCN	C2N+	N2			3.00E-10	0.00E+00	0.00E+00
N+	NCCN	C2N2+	N			1.40E-09	0.00E+00	0.00E+00
N2H+	NCCN	HNCCN+	N2			1.20E-09	0.00E+00	0.00E+00
HNCHCN	H+	HNCHCN+	H			4.00E-09	-5.00E-01	0.00E+00

Table 2. Table of the newly added ion-molecule reactions and charge exchange reactions

((McElroy et al., 2012; Wakelam et al., 2017; Manion et al., 2015).

Reactions					**α**	**β**	**γ**
CH3	NH	H	CH2NH		1.30E-10	1.70E-01	0.00E+00
CH3	NH	N	CH4		0.00E+00	0.00E+00	0.00E+00
CH	NH3	NH	CH3		8.00E-12	-5.00E-02	0.00E+00
CH	NH3	H	CH2NH		1.52E-10	-5.00E-02	0.00E+00
CH	NH3	H	H2	HCN	0.00E+00	0.00E+00	0.00E+00
C	CH2NH	CH2	HCN		1.00E-10	0.00E+00	0.00E+00
C	CH2NH	H	H2CCN		1.00E-10	0.00E+00	0.00E+00
CH2NH2	H	H2	CH2NH		3.00E-12	0.00E+00	0.00E+00
CH2NH2	H	NH2	CH3		1.07E-10	0.00E+00	0.00E+00
CH2NH2	O	OH	CH2NH		1.00E-11	0.00E+00	0.00E+00
CH2NH2	O	NH2	H2CO		1.00E-11	0.00E+00	0.00E+00
CH2NH2	N	NH	CH2NH		4.00E-11	1.70E-01	0.00E+00
CH2NH2	N	HCN	NH3		6.00E-11	1.70E-01	0.00E+00
H2CN	O	H2	OCN		0.00E+00	0.00E+00	0.00E+00
H2CN	O	OH	HCN		4.00E-11	0.00E+00	0.00E+00
H2CN	O	OH	HNC		1.00E-11	0.00E+00	0.00E+00
H	H2CN	H2	HNC		1.20E-11	0.00E+00	0.00E+00
CH3	N	H	H	HCN	6.00E-12	1.70E-01	0.00E+00
CH3	N	H	H2CN		5.60E-11	1.70E-01	0.00E+00
CH3	N	H2	HCN		0.00E+00	0.00E+00	0.00E+00
H2CN	N	NH	HCN		5.00E-12	0.00E+00	0.00E+00
H2CN	N	N2	CH2		4.00E-11	0.00E+00	0.00E+00
C2H5	N	CH3	H2CN		6.00E-11	1.70E-01	0.00E+00
C2H5	N	NH	C2H4		4.00E-11	0.00E+00	0.00E+00

C	H2CN	H2	CCN		3.00E-11	0.00E+00	0.00E+00
C	H2CN	CH	HCN		3.00E-11	0.00E+00	0.00E+00
C	H2CN	H	HCCN		3.00E-11	0.00E+00	0.00E+00
CH2	NH	H	H2CN		3.00E-11	0.00E+00	0.00E+00
CH2	NH	H	H	HCN	3.00E-11	0.00E+00	0.00E+00
CH2	NH	H2	HNC		3.00E-12	0.00E+00	0.00E+00
H2CCN	N	CN	H2CN		6.00E-11	1.70E-01	0.00E+00
CH3OCH2	N	H2CN	CH3O		3.00E-11	0.00E+00	0.00E+00
C	NH3	H2CN	H		6.70E-11	-5.10E-01	0.00E+00
CN	CH2NH	HNCHCN	H		4.59E-10	1.53E-01	8.71E-02
C2H3	N	H	H2CCN		6.40E-11	1.70E-01	0.00E+00
C2H3	N	NH	C2H2		1.30E-11	1.70E-01	0.00E+00
C	H2CCN	H	HC3N		1.00E-10	0.00E+00	0.00E+00
CH3	CN	CH2	HCN		0.00E+00	0.00E+00	0.00E+00
CH3	CN	H	H2CCN		1.00E-10	0.00E+00	0.00E+00
H2CCN	O	CH2	OCN		0.00E+00	0.00E+00	0.00E+00
H2CCN	O	CN	H2CO		1.00E-11	0.00E+00	0.00E+00
H2CCN	O	HCN	HCO		1.00E-11	0.00E+00	0.00E+00
H2CCN	O	H	CO	HCN	2.00E-11	0.00E+00	0.00E+00
C3N	O	CO	CCN		1.00E-10	0.00E+00	0.00E+00
CCH	N	H	CCN		1.50E-10	1.70E-01	0.00E+00
CCH	N	C	HCN		8.00E-12	1.70E-01	0.00E+00
CCH	N	C	HNC		2.00E-12	1.70E-01	0.00E+00
CCN	N	CN	CN		1.00E-10	0.00E+00	0.00E+00
C3N	N	CN	CCN		9.00E-11	1.70E-01	0.00E+00
CCN	O	CN	CO		7.00E-11	1.70E-01	0.00E+00
C	CCN	C2	CN		2.40E-10	0.00E+00	0.00E+00
C	C4N	C2	C3N		8.00E-11	0.00E+00	0.00E+00
C	C4N	CCN	C3		8.00E-11	0.00E+00	0.00E+00
C	C4N	CN	C4		8.00E-11	0.00E+00	0.00E+00
CH3O	O	OH	H2CO		6.00E-12	0.00E+00	0.00E+00
CH3O	O	O2	CH3		1.90E-11	0.00E+00	0.00E+00
CH3OH	OH	H2O	CH2OH		3.10E-12	0.00E+00	3.60E+02
CH3OH	OH	H2O	CH3O		6.00E-13	-1.20E+00	0.00E+00
CH3O	H	H2	H2CO		3.00E-11	0.00E+00	0.00E+00
CH3O	H	OH	CH3		3.00E-12	0.00E+00	0.00E+00
C	CH3O	CO	CH3		3.00E-10	0.00E+00	0.00E+00
CH3O	N	NH	H2CO		1.00E-11	1.70E-01	0.00E+00
CH3O	N	NO	CH3		3.00E-11	1.70E-01	0.00E+00

CH3OH	CN	HCN	CH3O		6.00E-11	0.00E+00	0.00E+00
CH3OH	CN	HCN	CH2OH		6.00E-11	0.00E+00	0.00E+00
S	CH3O	SO	CH3		4.00E-11	0.00E+00	0.00E+00
CCN	H	C	HCN		2.00E-10	0.00E+00	0.00E+00
CH	HCN	H2	CCN		1.40E-10	0.00E+00	0.00E+00
CH	HCN	H	HCCN		0.00E+00	0.00E+00	0.00E+00
CH	HNC	H2	CCN		1.40E-10	0.00E+00	0.00E+00
CH	HNC	H	HCCN		0.00E+00	0.00E+00	0.00E+00
S	CCN	CN	CS		7.00E-11	0.00E+00	0.00E+00
S	C3N	CS	CCN		1.00E-10	0.00E+00	0.00E+00
CH3OCH2	H	CH3	CH3O		3.00E-11	0.00E+00	0.00E+00
CH3OCH2	O	H	HCOOCH3		2.56E-10	1.50E-01	0.00E+00
C	CH3OCH2	C2H2	CH3O		3.00E-10	0.00E+00	0.00E+00
C	HNCS	CS	HNC		1.00E-10	0.00E+00	0.00E+00
C	HNCS	CS	HCN		1.00E-10	0.00E+00	0.00E+00
NH	HCS	H	HNCS		5.00E-11	0.00E+00	0.00E+00
CS	NH2	H	HNCS		1.00E-12	0.00E+00	6.00E+02
CH3	CH3OCH3	CH4	CH3OCH2		4.35E-14	2.68E+00	4.19E+03
C3	CH	H	C4		3.96E-10	0.00E+00	0.00E+00
C3	CH	C2	CCH		4.00E-11	0.00E+00	0.00E+00
C2	CH	H	C3		6.30E-11	0.00E+00	0.00E+00
C2	CH	C	CCH		3.70E-11	0.00E+00	0.00E+00
O	HCNS	NS	HCO		5.00E-10	0.00E+00	0.00E+00
O	HCNS	SO	HCN		5.00E-10	0.00E+00	0.00E+00
CN	HNC	NCCN	H		2.00E-10	0.00E+00	0.00E+00
CN	HNC	NCCN	H		2.00E-10	0.00E+00	0.00E+00

Table 3. Table of the newly added neutral-neutral reactions gathered from multiple databases, along with their respective α, β, and γ values ((McElroy et al., 2012; Wakelam et al., 2017; Manion et al., 2015).

Reactions					**α**	**β**	**γ**
HNCSH+	E	HS	HNC		5.26E-08	5.00E-02	0.00E+00
HNCSH+	E	H	HNCS		2.73E-08	5.00E-02	0.00E+00
HNCSH+	E	H	NCSH		1.16E-08	5.00E-02	0.00E+00
HNCSH+	E	S	H2CN		7.09E-11	5.00E-02	0.00E+00
HNCSH+	E	CS	NH2		1.61E-10	5.00E-02	0.00E+00

H2NCS+	E	H	HNCS		7.84E-08	5.00E-02	0.00E+00
H2NCS+	E	S	H2CN		8.44E-10	5.00E-02	0.00E+00
H2NCS+	E	CS	NH2		1.92E-09	5.00E-02	0.00E+00
H2NCS+	E	HS	HNC		1.55E-08	5.00E-02	0.00E+00
H2NCS+	E	H	NCSH		3.40E-09	5.00E-02	0.00E+00
NCHCN+	E	CN	HCN		1.50E-07	-5.00E-01	0.00E+00
CH3CN+	E	H	H2	CCN	2.00E-07	-5.00E-01	0.00E+00
CH3CN+	E	CN	CH3		1.00E-07	-5.00E-01	0.00E+00
CH3CN+	E	H	H2CCN		2.00E-07	-5.00E-01	0.00E+00
CH3CN+	E	H	H	HCCN	3.00E-07	-5.00E-01	0.00E+00
CH3CNH+	E	H	H	H2CCN	8.00E-08	-5.00E-01	0.00E+00
CH3CNH+	E	H	CH3CN		1.30E-07	-5.00E-01	0.00E+00
CH3CNH+	E	HNC	CH3		6.00E-08	-5.00E-01	0.00E+00
CH3CNH+	E	HCN	CH3		6.00E-08	-5.00E-01	0.00E+00
HC2N+	E	CH	CN		1.00E-07	-5.00E-01	0.00E+00
HC2N+	E	H	CCN		1.00E-07	-5.00E-01	0.00E+00
CH2CN+	E	H2	CCN		0.00E+00	0.00E+00	0.00E+00
CH2CN+	E	H	H	CCN	2.00E-07	-5.00E-01	0.00E+00
CH2CN+	E	H	HCCN		3.00E-07	-5.00E-01	0.00E+00
H2SCN+	E	H	HSCN		1.60E-07	-5.00E-01	0.00E+00
H2SCN+	E	H	HNCS		1.40E-07	-5.00E-01	0.00E+00
H2SCN+	E	CN	H2S		2.00E-07	-5.00E-01	0.00E+00
H2SCN+	E	H	CN	HS	2.00E-07	-5.00E-01	0.00E+00
HCNSH+	E	H	HCNS		1.00E-07	-5.00E-01	0.00E+00
HCNSH+	E	HS	HCN		3.00E-07	-5.00E-01	0.00E+00
HCNSH+	E	H	CN	HS	2.00E-07	-5.00E-01	0.00E+00
HCNH+	E	H	H	CN	9.06E-08	-6.50E-01	0.00E+00
HCNH+	E	H	HCN		9.62E-08	-6.50E-01	0.00E+00
HCNH+	E	H	HNC		9.62E-08	-6.50E-01	0.00E+00
HNCS+	E	S	HNC		1.00E-07	-5.00E-01	0.00E+00
HNCS+	E	S	HCN		5.00E-07	-5.00E-01	0.00E+00
HNCS+	E	CS	NH		1.50E-07	-5.00E-01	0.00E+00
HNCHCN+	E	HNCCN	H		6.60E-07	-6.00E-01	0.00E+00
NCCN+	E	CN	CN		1.50E-07	-5.00E-01	0.00E+00
HNCCN+	E	HNC	CN		3.00E-07	-5.00E-01	0.00E+00
HNCHCN+	E	NCHCN	H		1.50E-07	-5.00E-01	0.00E+00
HNCCN+	E	NCCN	H		3.00E-07	-5.00E-01	0.00E+00

Table 4. Table of newly added dissociative recombination reactions obtained from multiple databases, along with their respective α, β, and γ values (McElroy et al., 2012; Wakelam et al., 2017; Manion et al., 2015).

Reactions			α	β	γ
NCCN	C2N2+	E	1.00E-11	0.00E+00	2.00E+00
NCCN	CN	CN	1.30E-17	0.00E+00	4.74E+00

Table 5. Table containing two newly added photo-dissociation reactions obtained from databases, along with their respective α, β, and γ values (McElroy et al., 2012; Wakelam et al., 2017; Manion et al., 2015).

Results

TIME STEP	FRACTIONAL ABUNDANCE	TIME (YEARS)
1	1.00E-40	0
2	9.65E-33	1
3	1.35E-31	1.78E+00
4	1.57E-30	3.16E+00
5	1.47E-29	5.62E+00
6	1.15E-28	1.00E+01
7	8.03E-28	1.78E+01
8	5.27E-27	3.16E+01
9	3.73E-26	5.62E+01
10	3.72E-25	1.00E+02
11	4.75E-24	1.78E+02
12	4.74E-23	3.16E+02
13	2.85E-22	5.62E+02
14	1.16E-21	1.00E+03
15	4.71E-21	1.78E+03
16	3.28E-20	3.16E+03
17	5.07E-19	5.62E+03
18	8.25E-18	1.00E+04

19	7.04E-17	1.78E+04
20	3.06E-16	3.16E+04
21	1.02E-15	5.62E+04
22	3.16E-15	1.00E+05
23	1.03E-14	1.78E+05
24	4.72E-14	3.16E+05
25	1.28E-13	5.62E+05
26	8.93E-14	1.00E+06
27	4.76E-14	1.78E+06
28	1.85E-14	3.16E+06
29	6.64E-15	5.62E+06
30	4.26E-15	1.00E+07

Table 6. The raw data of the simulation of the abundance of cyanomethanimine over time.

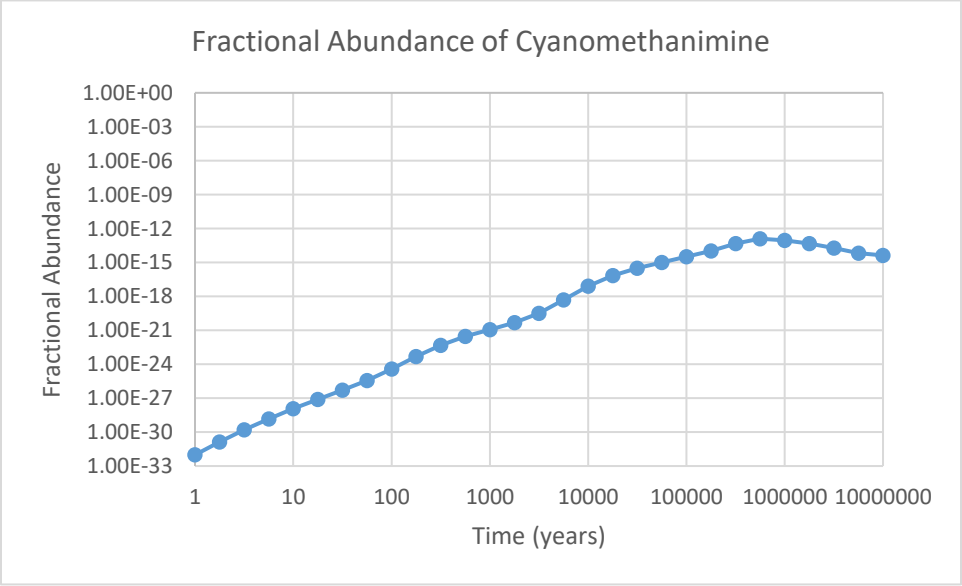

Figure 5. The fractional abundance of cyanomethanimine over millions of years, plotted on a logarithmic scale.

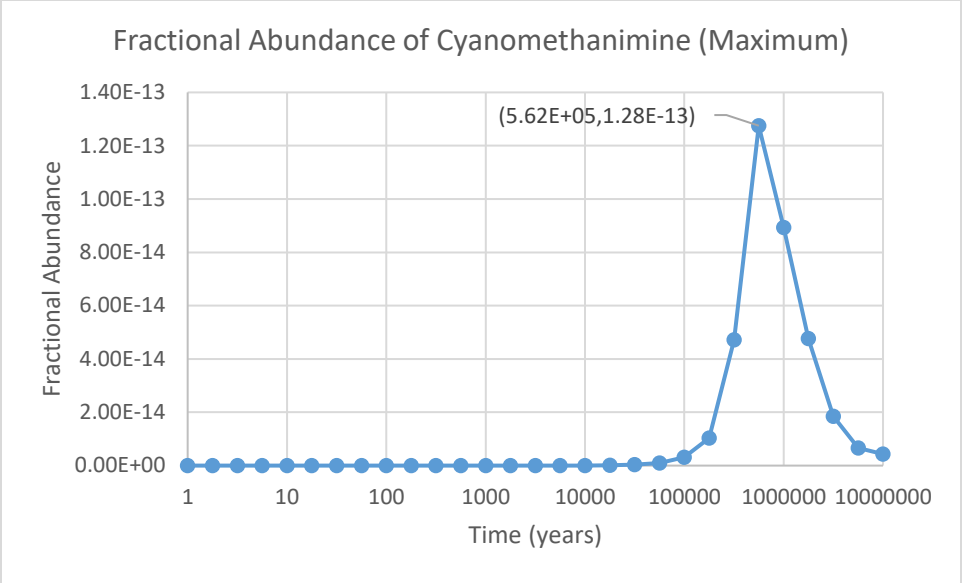

Figure 6. The fractional abundance of cyanomethanimine over time, plotted on a logarithmic x-axis only.

Discussion

The raw data points from the simulation are shown in Table 6, where the large changes in abundance over time can be seen numerically. The fractional abundance of cyanomethanimine was plotted against time, both of which were plotted on a logarithmic scale. Figure 5 shows a steady increase in cyanomethanimine abundance from 1 to 3.16 x 10^5 years, and a relatively steady slope from 1.78 x 10^6 years to 1.00 x 10^7 years. Figure 6 shows the maximum fractional abundance of cyanomethanimine to be 1.28 x 10^{-13} at 5.62 x 10^5 years. Compared to the maximum abundance of the similar prebiotic molecule ethanimine (Maximum abundance of around 10^{-12}) at the same conditions of 10 K and 2 x 10^4 cm^{-3}, cyanomethanimine is slightly less abundant at 1.28 x 10^{-13} (Quan et al., 2016). In the future, varying temperature and density should prove interesting when comparing

these two similar prebiotic molecules. It would be expected that an increase in temperature and/or density would lead to a sharper increase in maximum abundance of cyanomethanimine at a certain point in time, similar to ethanimine.

In order to improve the next round of results in the future, a few different ideas could be instated. The number of time steps could be increased so more points are available to plot, thus improving the resolution of each plot. The amount of time allotted to the simulation before "collapse" could be employed to allow for the analysis of the fractional abundances of cyanomethanimine over longer time periods. Adding grain reactions that are more closely related to cyanomethanimine could significantly impact the overall fractional abundances over time.

Conclusion

Cyanomethanimine was confirmed to reside in Sagittarius B2 through the comparison of spectra obtained in-lab and through the PRIMOS survey spectra (Zaleski et al., 2013). It is an important molecule to study due to its proposed importance in the synthesis of the nitrogenous base adenine (Roy et al., 2013). As a result, cyanomethanimine could play a critical role in the eventual formation of life. Sagittarius B2 is too distant to venture by spacecraft; Instead, computer modelling is the best method that currently exists in studying interstellar molecules. Computer simulations use the Arrhenius rate equation and differential equations to calculate fractional abundances of molecules with respect to hydrogen abundances.

The fractional abundance of cyanomethanimine at 10 K and 2 x 10^4 cm^{-3} is large and stable enough over time to continue studying its effects at varying temperatures and densities. Knowing a lot about cyanomethanimine's prevalence in interstellar medium will raise even more questions about both the origins of life of Earth and perhaps elsewhere in the vast expanses of the Universe.

Future Directions

The next step in studying cyanomethanimine in interstellar medium is to elucidate the effect of varying temperature and density on the abundance of the molecule. The study will likely involve computing abundances of cyanomethanimine at varying temperatures of 10 K, 50 K, and 90 K and at a constant density of 2 x 10^4 cm^{-3}. Additionally, temperatures of 10 K, 50 K, and 90 K will be input at densities of 2 x 10^5 cm^{-3} and 2 x 10^6 cm^{-3} so plots can be made with variable density at constant temperature and with variable temperature at constant density. It is expected that higher temperatures and densities will yield higher maximum abundances.

Subsequently, the E, Z, and N isomers of cyanomethanimine could be studied using computer modelling to determine individual abundances and how each isomer is impacted by varying temperature/density. The most stable isomer (Z-cyanomethanimine) is expected to be the most abundant. Studying each isomer is important because they have slightly different spatial arrangements that could create a difference in reactivity in each species. For example, Z-cyanomethanimine could be the most abundant in Sagittarius B2, but the E isomer could be more reactive and thus, more likely to form the

trimer of hydrogen cyanide aminomalononitrile. In other words, one isomer may be more favorable in the pathway to adenine than another.

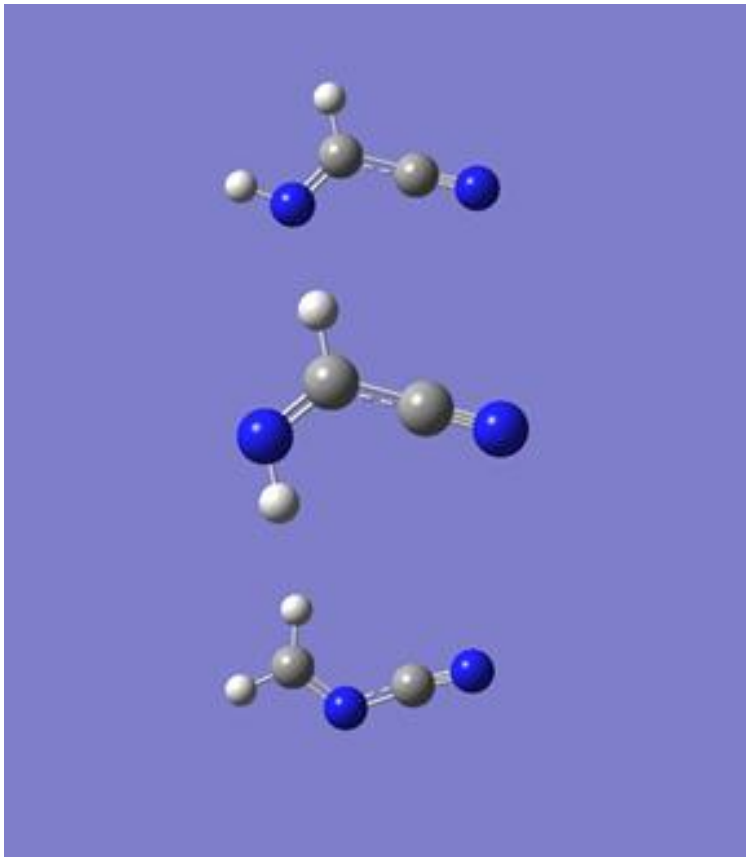

Figure 6. The isomers of cyanomethanimine. From top to bottom, the molecules are E-cyanomethanimine, Z-cyanomethanimine, and N-cyanomethanimine (Bailey, 2006).

Once cyanomethanimine is thoroughly studied, the trimer of hydrogen cyanide in the pathway of adenine, aminomalononitrile, could be studied if it is detected in Sagittarius B2 (Roy et al., 2013). Alternatively, other important precursors to biologically

significant molecules that are detected in Sagittarius B2 could be studied. For instance, precursors to cytosine, guanine, or uracil could be studied because they are equally important in the formation of RNA (and by extension, DNA) and for energy intensive processes that require ATP (adenosine triphosphate), GTP (guanine triphosphate), etc. (Berg, 2015).

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