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論文の要旨
Summary (Abstract) of doctoral thesis contents

Origin of life is one of the oldest mysteries for the mankind. According to a recent theory, complex organic materials might have been delivered to the primordial Earth by comets, and contributed to the chemical evolution leading to life. Therefore, the chemical evolution in the interstellar medium could be the very first stage of chemical evolution leading to life. In this thesis, I studied chemical evolution and chemical differences in hot cores via both observations and theoretical studies, especially focusing on N-bearing species, which can be related to the simplest amino acid, glycine.

I conducted a survey observation of CH_2NH, one of glycine precursors. As a result, I successfully detected CH_2NH toward eight hot core sources, including four new detections. Not only some well-known complex organic molecules, such as CH_3OH and CH_3OCH_3 but also N-bearing species, such as CH_2CHCN and NH_2CHO, were simultaneously detected. I found that chemical compositions are very different among the hot core sources. For instance, NGC6334F showed lower fractional abundances of CH_2NH and other N-bearing species than those in G10.47+0.03 by a factor of ten. Such differences would be reconciled by different evolutionary stages or different physical conditions of hot cores. I suggested two hypotheses to explain the chemical differences of the sources.

First, CH_2NH-rich sources might be in the early phase of the evolution. G10.47+0.03, one of the CH_2NH-rich sources, showed weak emission of hydrogen recombination line, and past high spatial resolution observation toward Orion KL “Hot Core” could not detect recombination lines inside it. On the other hand, NGC6334F and W51 e1/e2, where N-bearing species are not so rich, showed strong emission of a hydrogen recombination line emission, which would trace evolved HII region inside their hot cores. In this case, different fractional abundances might be explained by different strength of UV from central stars. If UV radiation is strong, molecules would be efficiently destroyed.

A second hypothesis is related to temperature structures inside the hot cores. According to a past study, G10.47+0.03 showed the highest gas kinetic temperature among the observed sources. If high temperature regions are limited inside NGC6334F and W51 e1/e2, CH_2NH and other species would be adsorbed on interstellar grains in their envelope.

To test above hypotheses, I conducted chemical network simulations. I used the dataset of KIDA (Wakelam et al. 2015), and some grain surface reactions were added taken from Garrod (2013). I assumed that physical evolution starts from a stage of the diffuse cloud will form a dense core via a gravitational collapse. Complex organic

molecules are formed in this cold phase on the grains. The gas kinetic temperature is assumed to rise after a birth of a star; then frozen solid-phase species are evaporated. Following that, evaporated species react with each other in the gas phase. These gas phase species in this stage are observed.

With our simulation, first of all, I revealed the formation paths to possible glycine precursors, CH_2NH and CH_3NH_2 with this modeling. I found that the hydrogenation processes to HCN is the most efficient way to produce CH_3NH_2. Then CH_3NH_2 is evaporated from grains after a birth of a star. On the other hand, CH_2NH is very poor on grains since CH_2NH is quickly converted to CH_3NH_2 via a hydrogenation process. I found that CH_2NH is formed in the gas phase via radical-radical reactions rather than direct evaporation from grains. This process starts with the evaporation of saturated molecules such as CH_3OH and NH_3, and they are destroyed to form radicals in the gas phase. Finally, NH and CH_3 radicals will efficiently form CH_2NH.

I also tested the hypotheses with this chemical model. First, I tested the effect of UV radiation. While grains would be destroyed by strong UV radiation in the vicinity of a star, UV radiation would be attenuated by grains outside of HII regions. Considering these effects and assuming a central B0 type star (T=30000 K), I found that gas phase species would be destroyed within 0.001 pc from an edge of HII regions, and the effect of UV is negligible further outside of this distance due to the strong attenuation by grains. The simulation results assuming UV radiation from well evolved HII regions succeeded to explain the observed abundances of CH_2NH toward NGC6334F and W51 e1/e2. These results agree with our observational results that strong hydrogen recombination lines were detected towards NGC6334F and W51 e1/e2. However, our simulation results under cases with different UV strength could not explain the different abundances of other detected species since they are destroyed more quickly than CH_2NH.

Second, I tested a possibility that different temperatures in hot cores may lead to the different chemical compositions. My model calculations suggested that N-bearing species such as CH_2NH and CH_2CHCN tend to be converted to other species on grains at or below 120 K after adsorption process, due to the longer timescale than 200 K case. On the other hand, CH_3OH, which did not show the correlation with CH_2NH, is not destructed on grains under 120 K. Therefore, the difference of the temperature among sources would be a possible explanation for the different CH_2NH abundance.

Finally, I discussed the formation process to glycine. I extended the work by Garrod (2013) by adding newly suggested formation processes to glycine and the latest gas phase reactions by KIDA. I confirmed that "CH_2NH_2 + HOCO" process, which was claimed by Garrod (2013), would be the most dominant formation process to glycine. However, while Garrod (2013) assumed that HOCO is formed by hydrogen subtraction processes from HCOOH, I found a more efficient formation path to the HOCO radical.

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I discussed the importance of suprathermal hydrogen, H*, which can penetrate high activation barrier with its excess energy given by UV photons. In this case, H* can react with a ubiquitous species, CO_2. I found that H* may accelerate the formation of HOCO via the reaction of “CO_2 + H*”. As the results, glycine abundance would be strongly enhanced.

Our simulations showed that CH_3NH_2 can be sufficiently formed on grains during the gravitationally collapse from the diffuse cloud phase and CH_2NH_2 is formed via hydrogen subtraction processes from CH_3NH_2. After that, the reaction of "CH_2NH_2 + HOCO" would form glycine efficiently in any star-forming regions. If glycine is sufficiently formed on grains, the aggregation of grains will form comets containing glycine inside. Such comets would have provided glycine to our primordial Earth and other exoplanets.

To further investigate this scenario, our next important step would be to achieve the first detection of interstellar glycine. Our simulations suggested that the UV photons from the central stars rather decreased glycine abundance since the destruction rates overcome the producing rates. It would be preferable to search for glycine in regions where UV radiation from central stars is well attenuated. The chemical simulations predicted that formation path of CH_2NH_2 would be hydrogen subtraction processes from CH_3NH_2, which would be abundant on the grains. Therefore, CH_3NH_2 would be a good compass to the first detection of glycine.

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博士論文審査結果の要旨
Summary of the results of the doctoral thesis screening

宇宙においてどのように生命が誕生したかを理解するうえで、生命関連分子の探査は宇宙物理学の最も重要なテーマの一つである。出願者は、もっとも簡単なアミノ酸であるグリシンに注目し、その前駆体である CH_2NH の観測的研究を行い、また、グリシンの生成メカニズムを考察した。

出願者は、まず、野辺山宇宙電波観測所の４５ｍ電波望遠鏡を用いて CH2NH およびその他の関連分子の探査を行い、８天体において CH_2NH の検出に成功した。そのうち、過去に検出の報告があるものが４天体、新たに検出されたものが４天体である。これまでにないサンプル数（８）をもとに CH_2NH の存在量の天体間での比較を行った。存在量には約１桁のレンジがあり、Orion KL (hot core) や G10.47+0.03 では多い一方、NGC6334F では存在量が低かった。水素結合線のデータとの相関を調べたところ、再結合線の強い天体では、CH_2NH の存在量が低い傾向があった。さらに、気相並びに固相の反応を含む化学反応ネットワークモデルによるシミュレーションを行い、CH_2NH の生成には固相反応よりも気相反応が重要であることを示した。ここまでの成果は、出願者が主著者の査読論文 Astrophysical Journal, 825, 79 としてすでに出版されている。

出願者はさらに、CH_2NH の存在量の天体間の違いを明らかにするため、化学反応シミュレーションによる研究を進めた。観測で示されたように、再結合線の強い天体では、CH_2NH の存在量が低い傾向があり、進化した HII 領域からの紫外線によって CH_2NH が壊されているらしいことが考えられた。別の可能性として、温度の高い領域が比較的小さい天体では、CH_2NH がよりダストに吸着されやすい可能性が考えられた。HII 領域の紫外線と温度の影響を探るために、簡単な分子雲の２層モデルを作成し、化学反応シミュレーションを行った。その結果､紫外線の効果のみでは存在量の違いを説明することはできないことが分かった。一方で化学反応シミュレーションでは、気相の CH_2NH が、120K より低温になるとダスト表面反応により壊されるようになる結果が得られ、温度の違いが観測された CH_2NH の存在量の違いに関係している可能性が示された。

出願者は、最後に、グリシンの生成メカニズムを検討した。CH_2NH_2 と HOCO ラディカルによる反応がグリシンの生成に最も有力であることが先行研究により示されていたが、出願者はさらに、紫外線によって余剰エネルギーを得た超熱的水素原子が HOCO の生成、ひいてはグリシンの生成を促進する可能性を提案した。本成果は、生命関連分子について観測及びシミュレーションを用いて研究を進め、興味深い結果を得たものであり、高く評価できる。

本研究で報告された観測は、出願者が自身で観測プロポーザルを準備し、観測・データ解析を主体的に行ったものである。また、化学シミュレーションも、研究に独自性を加え

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たものであり、高く評価される。したがって、審査委員全員が博士論文として合格であると判断した。