

Deuterium-Bearing Molecules in Cold and Warm Dense Interstellar Clouds

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Abstract. We have studied the production of key observed deuterium species for TMC-1, Orion, L134N and W3IRS4 clouds, of densities 104 cm^{-3} , 104 cm^{-3} , $5 \times 10^4 \text{ cm}^{-3}$, and 106 cm^{-3} respectively, by using the pseudo-time dependent gas-phase chemistry. These clouds have temperatures in the range 10-70 K. The main results by using the more extensive chemical network with the most updating reaction rates show that the most of calculated fractional abundances are in agreement with observations, and suggest that triply-deuterated ammonia could be detectable in dark clouds. Also our models show that large abundance of NH_2D and NHD_2 can be produced in the interiors of cold dense clouds at steady state time.

Introduction

Because deuterium-bearing molecules used to: probes of the physics of interstellar clouds, study the relation of connection between interstellar and cometary ices and understand the formation mechanism of isotopic composition of interstellar molecules ([1],[2],[3] and [4]). Therefore many theoretical and observational studies which have concerned on the formation of deuterated molecules in interstellar clouds.

In the last few years the studying of doubly-deuterated molecules in the interstellar medium has gained considerable attention. This is due to a large amount of doubly-deuterated formaldehyde, D_2CO , and ammonia, NHD_2 , have been observed towards low mass protostar IRAS16293-2422 ([5]), Orion cloud ([6]), very young protostellar core 16293E ([7]) and in the molecular cloud L1689N ([8], and [7]). Also NHD_2 observed in the molecular cloud L134N ([9]). While triply deuterated ammonia, ND_3 , observed in the low mass protostar NGC1333-IRAS4 ([4]), in the dark cloud B1 ([10]). But the methanol observed in the low mass protostar IRAS16293-2422 ([11]). All these observations suggest that deuteration of formaldehyde and methanol is produced during the cold and dense cloud ([12]).

There are two chemical networks for the formation of the deuterated molecules:

First, some deuterium-bearing molecules can be

formed by the gas-phase reactions, [13], [14], [1] and [2]. At the low temperatures 10-70 K, the H_2D^+ species is the key of gas-phase reaction to form DCO^+ and N_2D^+ , [4]. By gas-phase network [10] explained the observed abundance ratio of ND_3 in B1 cloud. Similarly [15] investigated the fractional abundance of NH_2D , which observed in L183 and TMC-1 clouds.

Second, the surface chemistry, in which deuterated molecules can be formed on dust grains. The high abundances of HDCO , D_2CO and CH_3OD in warm clouds are derived from the occurrence of grain surface chemistry during an earlier cold era followed by evaporation into the gas as temperature rise ([12], [16], [4] and [11]). The formation of singly and doubly deuterated isotopomers of formaldehyde and singly, doubly and multiply deuterated isotopomers of methanol on dust grain has been studied by [16], with a semi-empirical modified rate approach and Monte Carlo method in temperature rang 10-20 K.

In the present work, we shall confine ourselves to calculate the chemical abundances of key observed deuterium species, in several different interstellar clouds and comparison with both available observation and other theoretical models which are given for justification. This paper is organized as follow, in Section 2, chemical models are given. Sec., 3 contains a brief description of our gas phase chemical models. The conclusions are given in Sec. 4.

Chemical Models

In order to interpret the behavior of deuterium-bearing molecules on cold and warm interstellar clouds, we have carried a number of a pseudo-time dependent chemical models, which calculate the varying abundances of 408 species (130 of them containing deuterium) linked by 5320 reactions.

Our gas-phase model considers a standard gas-phase chemistry, in which we consider only reactions between gaseous species, with the exception that H₂ and HD forming on the grain surface, and we neglect the three body reactions.

[1] and [17] developed new models for the chemistry of deuterium, to investigate the fractionation of doubly-deuterated species, in interstellar molecular clouds. These models depend on a wide range of physical parameters including, density, temperature, elemental abundances and the freeze out of molecules on the dust grains. Our model is partially based on that part of gas-phase reactions of ([1] and [17]) for producing doubly-deuterated species. Our model extended the models of ([1] and [17]) to include multiply deuterated ammonia.

The mono-deuterated reaction set is complete in the sense that for every reaction containing a hydrogen-bearing molecule there is an analogue reaction containing the equivalent mono-deuterated species. If more than one reaction product contains hydrogen atoms then uncertainly arises as to which will be the deuterium bearing product. Due to lack of comprehensive experimental data, the usual approach is to assume statistical branching ratio between the various possibilities ([13] and [14]).

In this study we were interested in the chemistry of doubly deuterated ammonia, NHD₂. We also interested with multiply deuterated ammonia, which begin after the formation of NH₃, with deuterated ions XD⁺. In this model the metals (Fe, Mg, Na and Si) play an important role in determining the ionization fraction.

Since the chemical structure of interstellar clouds depends on the temperature, the radiation field and density number, then we have adopted four models of initial elemental (see table 1), to study the deuterium chemistry in TMC-1, Orion, L134N and W3 IRS4 clouds. We have neglected the chemistry of species of polycyclic aromatic hydrogen type and their reaction with smaller molecules. As [18] we also neglected the effects of enhanced rate coefficient in ion-polar neutral reactions. The chemical scheme used here is based on that of the most recent UMIST rate file, RATE99 [19], with updating the rate coefficients of some modifications

by [20]. We have adopted the cosmic D/H ratio measured by [21]. We used a constant ratio for C/O. we neglect the effect of X-ray ionization. The electron abundance is set equal to the sum of the ion abundances.

Table 1. Our Models, where n is number density

Model	n (m ⁻³)	T(k)	Average (mag.)	□□□□□
1		10	10	TMC-1
2	1.(4)	70	10	Orion
3	1.(4)	10	15	L134N
4	5.(4)	55	30	W3 IRS4

Results and Discussion

We have followed a large number of runs for the four models listed in Table (1). Using a different initial elemental abundances and cosmic ray ionization rate, the best initial elemental abundances are given in Table (2)..

Table 2. Initial fractional abundances

Species	Model 1	Model 2	Model 3	Model 4
H2	0.5	0.5	0.5	0.5
C+	7.3(-5)	7.3(-5)	7.3(-5)	4.0(-6)
O	1.7(-4)	1.7(-4)	1.7(-4)	8.0(-6)
N	2.14(-5)	2.14(-5)	2.14(-5)	5.1(-6)
S	1.0(-7)	1.0(-7)	1.0(-7)	6.0(-8)
Si	2.0(-8)	2.0(-8)	2.0(-8)	1.5(-10)
Fe+	1.0(-8)	1.0(-8)	1.0(-8)	1.5(-10)
Mg+	1.0(-8)	1.0(-8)	1.0(-8)	1.5(-10)
Na+	1.0(-8)	1.0(-8)	1.0(-8)	1.5(-10)
H3+	1.0(-11)	1.0(-11)	1.0(-11)	0.0
HD	1.6(-5)	1.6(-5)	3.2(-5)	5.0(-6)
He	0.14	0.14	0.14	0.14

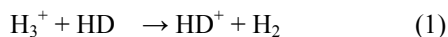
The cosmic ray ionization rate of $1.3 \times 10^{-17} \text{s}^{-1}$ is used for models (1-3) and high cosmic ray ionization rate of $1.3 \times 10^{-16} \text{s}^{-1}$ is used for model (4). The reduction of the initial elemental abundances and a high cosmic ray ionization rate used in model (4) is in agreement with [22].

Tables 3-6 compare the molecular D/H ratios observed toward the above four clouds, with the results from our gas-phase models at both early (10^5 year) time and steady state (100 million year) time, and other theoretical calculations

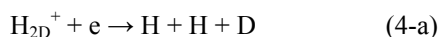
Table 3. A comparison of abundance ratio measured in TMC-1 cloud with predictions from our model (1) and [1]

Species	observ ation	Our cal. M1		RM 2000		REF
		Early steady	Early steady	Early steady	Early steady	
DCO ⁺ /H CO ⁺	0.02	0.01 8	0.08 2	0.01 9	0.08 7	15
NH ₂ D ⁺ /N H ₃	0.009- 0.014	0.08 6	0.02 9	0.08 4	0.02 8	15
HDCO/ H ₂ CO	0.0059- 0.11	0.04 3	0.05 6	0.04 2	0.05 5	33
DCN/H CN	0.023	0.00 6	0.02 2	0.00 9	0.02 5	33
DNC/H NC	0.015	0.01 5	0.01 5	0.01 5	0.01 5	34
C ₂ D/C ₂ H	0.01	0.01 2	0.02 8	0.01 1	0.02 7	13
C ₄ D/C ₄ H	0.004	0.00 4	0.02 7	0.00 4	0.02 9	35
N ₂ D ⁺ /N ₂ H ⁺	0.08	0.03	0.05 8	0.02 5	0.02 5	15
C ₃ HD/C ₃ H ₂	0.08- 0.16	0.00 7	0.02 7	0.00 6	0.02 6	26
C ₃ H ₃ D/C H ₄	0.054- 0.065	0.08 2	0.09 8	0.08 3	0.09 9	36
DC ₃ N/H C ₃ N	0.03- 0.1	0.00 8	0.02 6	0.00 7	0.02 6	37
DC ₃ N/H C ₃ N	0.013	0.02 3	0.02 6	0.02 3	0.02 6	38
HDCS/H CS	0.02	0.04	0.05	0.04	0.04 6	39

The most important primary reactions to extract deuterium from HD involve ion-neutral isotope exchange reactions:



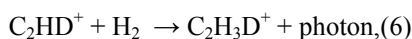
Where the reaction exoergicities although small - $\Delta E_1/k = 220 \text{ K}$, $\Delta E_2/k = 375 \text{ K}$, $\Delta E_3/k = 550 \text{ K}$ - are much larger than the temperatures of cold interstellar clouds. At low temperatures, the reverse reactions do not occur efficiently despite the large abundance of H₂. Once formed these deuterated ions can pass on their enhanced deuterium content to other species in chemical reactions, [23]. In addition to the forward and reverse reaction in (1), H₂D⁺ can be destroyed by metals, by dissociative recombination with electron,



With total rate coefficient equal to $6 \times 10^{-8} (T/300)^{-0.5} \text{ cm}^3 \text{ s}^{-1}$, [24] and by reaction with neutral molecules

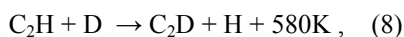
(CO, N₂, H₂D).

The reactions for CH₂D⁺ and C₂HD⁺ are similar to that of H₂D⁺, except that each of these ions undergo a radiative association reaction with H₂ ([13] and [25])

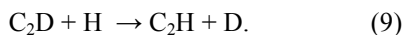


Our calculated ratios for H₂D⁺/H₃, CH₂D⁺/CH₃⁺ and C₂HD⁺/C₂H₂⁺ are all enhanced at low temperature, but H₂D⁺ is responsible for D/H ratio other than the two molecules. At high temperature H₂D⁺ is rapidly destroyed by H₂, so CH₂D⁺ and C₂HD⁺ are responsible for D/H ratio.

Our calculated ratio of C₂D/C₂H is in agreement with observations of TMC-1 at an early (10⁵ year) time and higher at the steady state (10⁸ year) time. This result is the same as that obtained by [1]. The C₂D species is formed by:



and is destroyed by



In model (2) with temperature of 70 K, the neutral-neutral rate coefficient of reaction (8) and dissociative recombination of C₂HD⁺, become more competitive, and fractional abundance of C₂D increases. This result agrees with that of [25]. Also C₂D is formed from cosmic ray induced photodissociation of C₂HD. At steady state time our calculated C₂D/C₂H ratio is in agreement with observations of Orion cloud and greater than that obtained by [13].

As [13] C₂H₃D⁺ is precursor to C₂H₂D, so the reactions of C⁺ with C₂H₂D transfer fractionation to C₃-bearing hydrocarbons via



and subsequently to C₃D via dissociative recombination. The C₃H₂ molecule is not transferred easily to the C₃HD⁺ and C₃HD is formed as (see [26]);

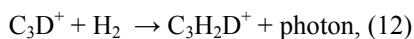


Table 4. A comparison of abundance ratio measured in Orion cloud with predictions from our model (2) and [13]

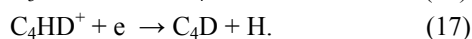
Species	observ ation	Our cal. M2	M1998	REF
DCO ⁺ /HC O ⁺	0.002	0.002	8.(-4)-8.(-5)	40
NH ₂ D/NH ₃	0.003	0.0029	4.(-4)	45
HDCO/H ₂ C O	0.02	0.019	0.004-0.005	44
DCN/HCN	0.006	0.0058	0.001-4(-4)	34
DNC/HNC	0.01	0.043	9.(-4)-2.(-4)	34
C ₂ D/C ₂ H	0.045	0.032	0.003	42,43
CH ₃ OD/CH ₃ OH	0.01- 0.06	0.005	0.003-0.004	46
HDO/H ₂ O	>0.002	0.001	0.001-2.(-4)	47

Note : a(-b) stands for $a \times 10^{-b}$

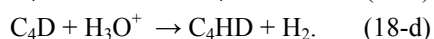
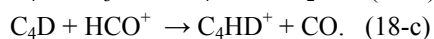
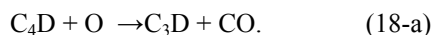
Our calculated C₃HD/C₃H₂ ratios in the both an early and the steady state times are not in agreement with observation of TMC-1 cloud.

In our model C+3H₃D molecule is formed through the CH₂D⁺ ion, by dissociative recombination of CH₂DC₂H₂⁺ and CH₂DC₃H₂⁺ ions, which are themselves formed from CH₂D⁺ by ion-neutral reactions with small hydrocarbon species like methane or acetylene. C₃H₃D is destroyed by atomic and molecular ions, primarily H₃⁺ and He⁺. Our calculated C₃H₃D/C₃H₄ ratios at an early and the steady state time are greater than the lower and upper limit of observations of TMC-1 cloud. This results is the same as that of [1].

In our model C₄D species is formed by the following reactions :



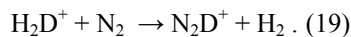
and is destroyed by



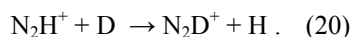
At an early time our calculated C₄D/C₄H ratio is in agreement with observations of TMC-1 clouds.

The D-N bond begins due to the lower proton

(deuteron) affinity of H₂D⁺, which reacts with N₂ to form N₂D⁺ species,



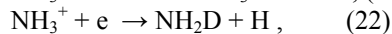
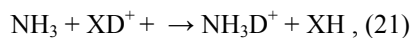
In addition to reaction (19), D atom can also react with N₂H⁺ to form N₂D⁺



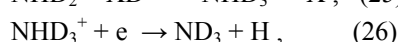
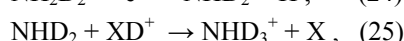
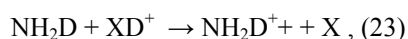
Reaction (20) has an exothermicity of about 550 K , [27]. Due to the proton affinity of N₂ is very small, so that N₂D⁺ reacts with CH₂D⁺ and C₂HD⁺.

IN our model N₂D⁺/N₂H⁺ ratios are less than the observations of TMC-1 and Orion clouds. This is because at dense clouds N₂D⁺ condense onto grains, i.e. N₂D⁺ is not easily predictedable by gas-phase reactions and its value must be predicted through evaporation from the grain ([28], [13] and [23])

After NH₃ is formed by the reaction sequence $N_2 \xrightarrow{He^+} N^+ \xrightarrow{4H_2} NH_4^+ \xrightarrow{e} NH_3$, deuteron transfer reaction forms NH₃D⁺ which can then recombine to give NH₂D as;



where XD⁺ represents all species capable of transferring a proton or deuteron to NH₃, principally H₃⁺, N₂H⁺, HCO⁺ and their deuterated isotopomers. Successive deuteron transfer reaction can lead eventually to NHD₂ and ND₃ as



From the last reactions (21-27) the relative fractional abundances depend on the XD⁺/XH⁺ and the branching ratio for dissociative recombination of the deuterated ions.

By assuming the rate coefficients of reactions (26) and (27) are equal, our calculated fractional abundances for ND₃ is about 2×10^{-11} . This value is greater than that obtained by [29] by two times. The abundance of ND₃ in our model is in the same order of magnitude as given by [10] for B1 cloud. From this result we can conclude that ND₃ can be detected in L134N cloud.

Table 5. A comparison of abundance ratio measured in L134N ([15] and [9]) with predictions from our model (3) and [23]

Species	observation	Our cal. M2		M2002	
		early	steady	early	steady
DCO ⁺ /HCO ⁺	0.18	0.026	0.17	0.016	0.047
NH ₂ D/NH ₃	0.1	0.006	0.1	0.0075	0.02
NHD ₂ /NH ₃	5.(-3)	2.3(-5)	5.1(-3)	1.3(-4)	8.4(-5)
N ₂ D ⁺ /N ₂ H ⁺	0.35	0.03	0.038	0.023	0.039

One species for which time dependence significant is DCO⁺. The species DCO⁺ is more readily observable than N₂D⁺, because the abundance of CO is greater than that of N₂ in interstellar clouds. So at low temperature the D-C band begins with the reaction:



at an early time. Also DCO⁺ is formed by:

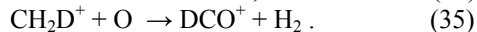
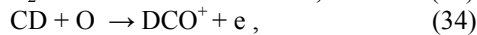
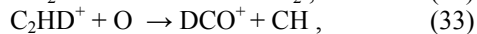
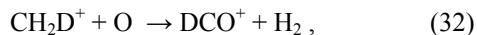


At the low temperature and density, the atomic deuterium is very abundant, so reaction (30) proceeds very rapidly and can further enhance the fractionation of DCO⁺.

At high temperature the abundance of CH₄D⁺ is greater than H₂D⁺, then DCO⁺ is formed by,



In addition to this reaction, there are significant contributions to DCO⁺ formation in the reactions

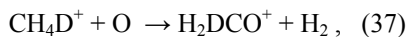


The primary of D in dark clouds is the dissociative recombination of DCO⁺,



Our calculated DCO⁺/HCO⁺ ratio is in agreement with observations of TMC-1 cloud at an early time. At the steady state time it is in agreement with observations of Orion and L134N clouds. This result differs than that obtained by [13] and [23].

The band between D-C-O begins by the formation of deuterated formaldehyde, HDCO, which is formed from two species derived from CH₂D⁺, CH₄D⁺ and CH₂D, via the reactions;



followed by dissociative recombination



and



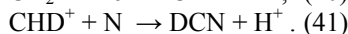
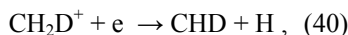
HDCO also reacts with H₃⁺ to form H₂DCO⁺ which will then recombine to HDCO. The calculated HDCO/H₂CO ratio is in agreement with observations of TMC-1, Orion and W3IRS4 clouds.

Table 6. A comparison of abundance ratio measured in W3IRS4 cloud by [48] with predictions from our model (4)

Species	observation	Our cal. M2
HDS/H ₂ S	<9.1(-2)	1.0(-3)
HDCO/H ₂ CO	<3.8(-2)	0.02
DCN/HCN	<4.3(-3)	0.001
DNC/HNC	7.1(-3)	9.(-4)
C ₂ D/C ₂ H	0.045	0.032
CH ₃ OD/CH ₃ OH	<7.1(-2)	0.006

Note: a(-b) stands for ax10^{-b}

Also the band between D-C-N begins by the formation of DCN, which is formed a derivative of CH₂D⁺;



The main derives of DCN at high temperature is the neutral-neutral reactions;



We found that the reaction

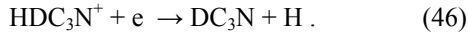


can cycle deuterium between the atomic D and the DCN molecule. This result is in agreement with that of [30] and [31]. As shown in tables (3, 4 and 6) our calculated DCN/HCN is in agreement with observations of TMC-1, Orion and W3IRS4 clouds.

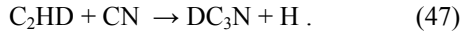
At the low temperature, the dominant route to deuterated cyanoacetylene, DC₃N, formation is thought to be



followed by

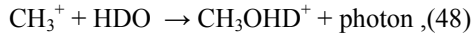


At the high temperature, the deuterated acetylene should form deuterated cyanoacetylene through

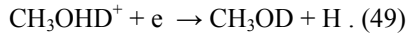


DC_3N species is only observed in TMC-1 cloud, and our calculated its ratio is in agreement with observations at steady state time.

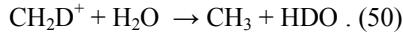
In our models we have assumed that the species CH_3OD is formed from the radiative association reaction



and

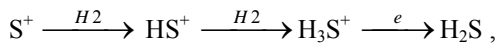


The HDO species comes from the rapidly exothermic reaction

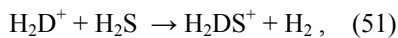


The calculated $\text{CH}_3\text{OD}/\text{CH}_3\text{OH}$ ratio in our model differs from observations. This is because, at high densities most molecules condense onto grain; i.e. CH_3OH and CH_3OD is not easily predictable by gas-phase reaction and their values must be predicted through evaporation from the grains surface, [22]. Also our calculated ratio for $\text{HDO}/\text{H}_2\text{O}$ is small, because the large value must be predicted by shock chemistry, [32] and [11].

When we compare our predicted gas-phase abundances with those observed in TMC-1 and W3IRAS4 clouds, only HDCS is in agreement and other species HDS is smaller than observation. In our model after the formation of H_2S by the chain;

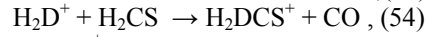
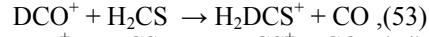


(By the last chain the calculated fractional abundance of H_2S is small) deuteron transfer reaction forms H_2DS^+ which then recombine to give HDS as :



Also DCO^+ and H_2D^+ react with H_2CS to form HDCS

as;



Conclusions

With a more extensive chemical network, we made a detailed study of a pseudo-time dependent chemical evolution of deuterium species in different interstellar clouds, TMC-1, Orion, L134N and W3IRS4, with different densities and temperatures. This has been done using different initial elemental abundances and without the temperature dependence of the ion-dipole molecule collisions. We have shown that large abundances of NH_2D and NHD_2 can be produced by gas phase chemistry in cold dense clouds. Ammonia is deuterated via deuteron transfer from species such as H_2D^+ , DCO^+ and N_2D^+ , followed by dissociative recombination. We predict the abundance of ND_3 is 2×10^{-11} , by assuming the rate coefficients of reactions $\text{NHD}_3^+ + e \rightarrow \text{ND}_3 + \text{H}$, and $\text{NHD}_3^+ + e \rightarrow \text{NHD}_2 + \text{D}$ are equal. So we suggest that triply-deuterated ammonia could be detectable in L134N cloud. We have included the fractionation of sulphur-bearing molecules and found a good agreement with observation for HDCS. The very slow formation rates of HDS in cold gas make this molecule particularly useful in probing regions where grain surface chemistry may be important. Reduction of the initial elemental abundances and high cosmic ray ionization gave us good relative abundances for most of the observed deuterated species in W3IRS4.

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احتراق جزيئات الديوتريوم في السحب البين نجمية الكثيفة الباردة والدافئة

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(قدم للنشر في ٢٤/٢/١٤٢٩هـ؛ وقيل للنشر في ٤/٧/١٤٢٩هـ)

ملخص البحث. حيث أن جزيئات الديوتريوم تستخدم في: ١- اختبار القوانين الفيزيائية لسحب ما بين النجوم. ٢- دراسة علاقة الربط بين تكوين الثلج في مادة ما بين النجوم والمذنبات. ٣- طريقة تكوين نظائر المركبات في مادة ما بين النجوم. لهذا تقوم دراسات نظرية وعملية (عن طريق رصد السحب البين نجمية بطرق مختلفة)، لفهم عملية تكوين وتكوين مركبات الديوتريوم وحساب كمية الوفرة في سم^١. في هذا البحث نقوم بدراسة طريقة تكوين مركبات الديوتريوم وحساب كمية الوفرة في أربعة سحب بين نجمية ذات عوامل فيزيائية مختلفة وهي TMC-1 و Orion و L134N و W3IRS4. وفي هذه الدراسة تم تسيد برنامج كيميائي يحتوي على ٥٣٤٠ تفاعل كيميائي لـ ٤٠٨ مركب وعنصر كيميائي منهم ١٣٠ مركب للديوتريوم. وقد تم تحويل هذه التفاعلات إلى معادلات تفاضلية من الدرجة الأولى تحقق شرط stiff وحلها عددياً باستخدام طريقة الـ Gear. وقد تم الحصول على قيم متوافقة مع الأرصاد الفلكية باستخدام قيم بدائية مختلفة للعناصر الأساسية حسب الوضع الفيزيائي للسحابة المدروسة. وقد تم الحصول على قيم وفرة كبيرة لكل من NH₂D و NHD₂ في السحب الكثيفة الباردة عند حصول حالة الثبات في عملية التكوين والتكسير عند زمن قدرة مائة مليون سنة.