

# Gas-Grain Chemistry of NGC 2264 IRS1 Dense Cloud

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We have studied the chemistry of NGC2264 IRS1 cloud. The chemical evolution is studied using Pseudo-time-dependent of gas phase and gas-grain chemistry with thermal desorption. Our results confirm the importance of grain chemistry in predicting the observed species in NGC2264 IRS1 at the reduction of H<sub>2</sub> formation rate on grain surface

*Key words:* Astrochemistry,

## 1. Introduction:

Young stars have a significant impact on the chemistry in the dense molecular clouds, in which they form. This is true for hot cores, where high temperatures and densities act to drive a rapid chemistry (Hatchell et. al 1998 and Charnley 1997). The raised temperature releases molecules from the icy mantles on grains and so provide fuel for chemical network (Buckle and Fuller 2002).

The star forming region NGC2264 is a young open cluster of the age of about three million years at a distance of 800pc from the Sun. The near-infrared source IRS1 is the brightest IRAS source (2300L<sub>0</sub>) in NGC2264 (Nakano et. al 2003). NGC2264 IRS1 was one of the good sites for the study of cluster star formation and many observational works have been made (Schwartz et. al 1985, Krugel et. al 1987 and Phillips et. al 1988). Schreyer et, al (1997) have performed an infrared imaging at J, H and K bands using the MAGIC (Black)- camera for NGC2264 IRS1 molecular cloud and found the physical conditions as temperature  $T(k) = 55^{+20}_{-10}$  and density  $n(H_2) = (2-3) \times 10^6 \text{cm}^{-3}$ .

Significant works have been involved in developing an understand of the chemistry of star forming regions. This ranges from studies of cold, dark clouds (e.g. Herbst. and Klemperer 1973, Prasad and Huntress 1980, Leung, et al 1984, Amin 1999, Gwelan et. al 2000 and Amin and El-Nawawy 2004, 2005) to hot cores (e.g. Millar 1993, Walmsley and Schilke 1992, Kurtz et. al 2000). In these studies the chemistry is considered for a homogeneous cloud, or a point within a cloud.

In the present work, we focus on the chemical evolution of NGC2269 IRS1. The main objective of the present work is to obtain the key of observed abundances, which were obtained by Schreyer et al (1997). The species abundances will be calculated by using the gas-grain chemistry at different grain temperature, assuming different initial elemental abundance. Comparisons with both available observations and other theoretical models are given for justification. This paper is organized as follows in section 2, chemical models are given. Section 3 contains a brief description of our gas-grain chemical models. The Conclusions are given in section 4.

## **2 The Models**

### **2.1 Gas Phase Chemistry:**

We have constructed a model to study NGC2264 IRS1. We have carried a number of pseudo-time dependent chemical models, which are calculated by varying the abundances of 278 species linked by 3061 reactions. Our gas-phase model considers standard gas-phase chemistry, neglecting the three body reactions. The chemical scheme used is based on that of Amin(2000), Amin and El-Nawawy (2005) and UMIST rate file, RATE99 (Le Teuff et al 2000). The cosmic ray ionization rate is assumed to be  $1.3 \times 10^{-17} \text{ s}^{-1}$ . We neglect the effect of X-ray ionization. The electron abundance is set equal to the sum of the ion abundances.

Since the chemical structure of interstellar clouds depends on the temperature, the radiation field and density number, we have adopted the physical parameters obtained by Schreyer et al (1997), (i.e. temperature  $T = 55\text{K}$  and number density  $n = 2 \times 10^6 \text{ cm}^{-3}$ ) to interpret the behaviour of the observed species in the NGC2264 IRS1. We have carried out four models and their physical parameters are given in Table (1).

**Table (1): Our Models**

<b>Model</b>	<b>T<sub>g</sub> (k)</b>	<b>T<sub>d</sub> (K)</b>	<b>Density (n) cm<sup>-3</sup></b>
M <sub>1</sub>	55	zero	2x10 <sup>6</sup>
M <sub>2</sub>	55	10	2x10 <sup>6</sup>
M <sub>3</sub>	55	55	2x10 <sup>6</sup>
M <sub>4</sub>	55	55	2x10 <sup>-6</sup>

Where T<sub>g</sub> and T<sub>d</sub> are the gas and grain temperatures

## 2.2 Grain Chemistry

Our chemical network contains 4571 reactions involving 419 species (141 grain surface species). The network of gas grain chemistry are developed using the data given by Hasegawa et al. (1992) and Hasegawa and Herbst (1993b). The chemical rate equation for a species I in the gas phase with concentration n(i) and on grain surface with concentration n<sub>s</sub>(i) (Hasegawa and Herbst 1993a) are given by

$$\frac{dn(i)}{dt} = \sum_l \sum_j K_{lj} n(j) n(l) + [K_{evap}(i) + K_{crd}(i)] n_s(i) - \dots n(i) \left[ \sum_j K_{ij}(j) + K_{acc}(i) \right] \dots (1)$$

$$\frac{dn_s(i)}{dt} = \sum_l \sum_i K_{jl} n_s(j) n(l) + K_{acc}(i) n(i) - \dots n(i) \left[ \sum_j K_{ij} n_s(j) + K_{evap}(i) + K_{crd}(i) \right] \dots (2)$$

Where K<sub>ij</sub> and K<sub>lj</sub> represent the gaseous and surface rate coefficients respectively, for reaction between species i and j. K<sub>acc</sub>(i), K<sub>evap</sub>(i) and K<sub>crd</sub>(i) are rates of accretion on grain surface, thermal evaporation and desorption by cosmic ray (s<sup>-1</sup>) for species i, respectively. We have added the following grain processes into the last rate file for gas-phase reactions: accretion on grain surface, surface reaction, cosmic ray

desorption, cosmic ray induced photo-desorptions and desorption by  $H_2$  formation.

The physics describing these processes are given by Leger et al (1985), Hartquist and Williams (1990), Willacy and Williams(1993), Hasegawa and Herbst(1993a and b), Shalabia and Green (1994) and Willacy and Millar(1998).

Collings et al. (2004) show that the thermal desorptions are complex processes. In our models we tack the simple formula for the thermal evaporation rate  $K_{evap}$  of the  $i$ th surface species which is given by Watson and Salpeter (1972) and Wiebe et.al (2003), as

$$K_{evap}(i) = v_0 \exp\left(-\frac{E_b(i)}{kT_d}\right) \dots(3)$$

Where  $T_d$  is the grain (dust) surface temperature,  $E_b$  is the binding energy for physical adsorption of the  $i$ th species to the dust surface and  $v_0$  is the characteristic vibrational surface for the adsorpted species given by equation (3) from Hasegawa et. al (1992). We assume that  $v_0=1 \times 10^{13} s^{-1}$  for all species. Values of  $E_b$  are taken from the table completed by Aikawa et al (1996) and Haseqawa and Herbst(1993b). Following Rodgers and Charnley (2003), we assume a neutral molecule

in our scheme is not on this list, we assume a default value for  $\frac{E_b}{k}$  of 4820K, which is equivalent to assuming that desorption is controlled by  $H_2O$ . In our model we neglect the non-thermal desorption of  $CO$ ,  $N_2$  and  $CH_4$ .

### 3. Results and discussion

We have followed a large number of trials before reaching to the most acceptable models discussed in section (2), by using different initial elemental abundances. The most fitting initial elemental abundances describe the gas-grain chemical abundance for the considered cloud is given in Table (2). In our models M1 and M2 the initial abundance of ionic and molecular species are taken equal to zero. We stopped the calculations at 3Myr, which is the age of NGC2264, Nakano et al. 2003. The sources of ionization in our models are both cosmic ray ionization and internal ultraviolet photons induced by cosmic ray.

**Table (2): Initial Elemental Fractional Abundances**

Species	Frac.	Species	Frac.
H <sub>2</sub>	0.45	Na <sup>+</sup>	$2 \times 10^{-9}$
H	0.1	Mg <sup>+</sup>	$7.9 \times 10^{-9}$
He	0.14	Si <sup>+</sup>	$0.5 \times 10^{-9}$
C <sup>+</sup>	$7.3 \times 10^{-5}$	S <sup>+</sup>	$2 \times 10^{-7}$
O	$1.67 \times 10^{-5}$	Fe <sup>+</sup>	$3 \times 10^{-9}$
N	$2.15 \times 10^{-5}$		

In general the chemical evolution resulting from the different models are compared with the observations of NGC2264 IRS1 and the results are shown in table (3).

**Table (3): Comparison of the results of our models with observations**

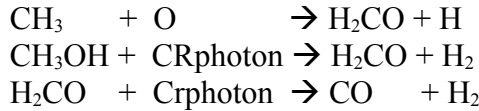
Species	observation	M1	M2	M3	M4
CS	1.3(-9)	1.0(-9)	1.2(-9)	1.2(-9)	1.2(-9)
CN	1.6(-9)	1.4(-9)	4.3(-10)	1.0(-9)	1.0(-9)
HCN	3.2(-9)	2.0(-9)	1.0(-9)	2.0(-9)	2.5(-9)
HC <sub>3</sub> N	2.4(-10)	1.0(-9)	1.3(-10)	1.0(-10)	2.0(-10)
NH <sub>3</sub>	1.2(-8)	2.0(-8)	1.4(-8)	2.0(-8)	3.0(-8)
C <sub>2</sub> H	9.0(-9)	8.0(-14)	1.5(-10)	4.0(-10)	3.0(-9)
H <sub>2</sub> CO	1.3(-10)	1.0(-10)	4.5(-10)	5.0(-10)	7.0(-10)
CH <sub>3</sub> OH	8.8(-9)	4.0(-13)	4.0(-10)	4.5(-10)	5.2(-9)
CH <sub>3</sub> CN	8.2(-11)	4.0(-14)	8.7(-12)	9.5(-12)	5.0(-11)
SO	9.2(-10)	3.0(-10)	1.0(-10)	5.0(-10)	8.0(-10)
SO <sub>2</sub>	2.0(-10)	1.0(-10)	4.0(-10)	1.0(-10)	1.7(-10)
SiO	4.7(-11)	1.1(-11)	2.0(-11)	3.0(-11)	4.0(-11)
HCO <sup>+</sup>	2.2(-9)	1.0(-10)	8.0(-10)	9.5(-10)	2.0(-9)

<b>HCS<sup>+</sup></b>	2.6(-11)	1.5(-12)	1.0(-12)	2.0(-11)	1.8(-11)
<b>N<sub>2</sub>H<sup>+</sup></b>	3.6(-10)	2.5(-12)	5.0(-11)	7.0(-11)	2.5(-10)

Where  $a(x) = ax10^x$

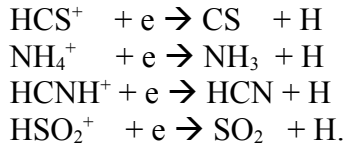
### 3.1 Gas-Phase model.

For gas-phase model (M1) eight species are in agreement ( i.e in the same order of magnitude) with observations,. Bergin (2002) suggested that H<sub>2</sub>CO is likely to be formed on grain surface. Our results of (M1) show that H<sub>2</sub>CO can be predicted by gas-phase model. This is because the main formation route of H<sub>2</sub>CO depends on Oxygen atoms and the destruction route depends on cosmic-ray photons as follows :

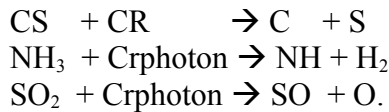


The chemical route of key observed species, which are in agreement with observations are:

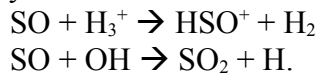
*First* - Dissociative recombination with electron is the main route of formation of CS, HCN, SO<sub>2</sub> and NH<sub>3</sub> through the following reactions:



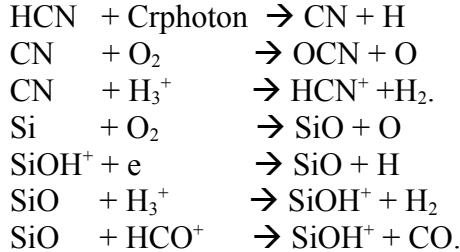
While the reactions with cosmic-ray photons and cosmic-ray induced photons are the main route of destructions as follow:



The last reaction is the main route of formation of SO molecule. The formation of SO by neutral-neutral reaction of S and O<sub>2</sub> is inefficient here, because it has energy barrier of 265K, Pineau des Forets et. al (1993) and Amin(1999). On the other hand the destruction of SO is given by :



*Second* - Both CN and SiO molecules in our model has a chemical route as follow:



From the last two reactions we see that  $\text{SiOH}^+$  return to react with electrons to form SiO.

### 3.2 Gas-Grain models.

It is generally believed that the relatively large abundances of hydrogenated , saturated , small molecular species and large complex molecules observed in NGC2264 IRS1, are related to the evaporation of grain mantle material.

The models M2, M3 and M4 are Gas-Grain models. In M2 the gas temperature differs from the grain temperature. In M3 and M4 the gas temperature is assumed equal to the grain temperature. The formation of  $\text{H}_2$  on grain surface differs in the two last models ( M3 and M4 ). In M3 and M4  $\text{H}_2$  formation rates are  $5.2 \times 10^{-17} (\text{T}_d \times 3.33 \times 10^{-3})^{0.5}$ , Amin and El-Nawawy (2005) and  $1.4 \times 10^{-17} (\text{T}_d \times 3.33 \times 10^{-3})^{0.5}$ , respectively.

**Table(4): Evaporation time ( $t_{\text{evap}}$ ) and critical temperature ( $T_{\text{crit}}$ )**

Species	$T_{\text{evap}}$ (sec)		$T_{\text{crit}}$ (K)
	$T_d = 10\text{K}$	$T_d = 55\text{K}$	
CS	very high	6.2(3)	43
CN	very high	7.0(-1)	32
HCN	very high	1.6(2)	38
$\text{HC}_3\text{N}$	very high	4.9(11)	64
$\text{NH}_3$	very high	4.9(-4)	23
$\text{H}_2\text{CO}$	very high	1.6(2)	38
$\text{CH}_3\text{OH}$	very high	3.8(4)	45
$\text{CH}_3\text{CN}$	very high	2.4(5)	47

SO	very high	6.2(3)	43
SO <sub>2</sub>	very high	3.0(12)	66
SiO	very high	4.3(15)	74
C <sub>2</sub> H	very high	7.0(-1)	32

Table (4) give us the evaporation time at  $T_d = 10\text{K}$ ,  $T_d = 55\text{K}$  and critical temperature for the key observed species in NGC2246 IRS1. From equation (3) we can calculate the critical temperature  $T_{\text{cirt}}$  at which the desorption time scale equals one year. It is easy to show that  $T_{\text{crit}} = E_b/47\text{K}$ .

Table (4) shows that for  $T_d = 10\text{K}$  all species has a long time of evaporation  $t_{\text{evap}}$ . The thermal desorption at this temperature is unimportant, this is in agreement with that of Hasegawa and Herbst (1992). For  $T_d = 55\text{K}$  most of the species has a small  $t_{\text{evap}}$ , except SiO molecule. So that most of the species are off the grain mantle at short time and the thermal desorption became an important in the gas-grain chemistry at high temperature.

In our model M2 by using the relation given by Nomura and Millar (2004) for the accretion time scale ( $3 \times 10^9/n \text{ (cm}^{-3}\text{)}$  at  $T=10\text{K}$ ) of gas-phase atoms and molecules onto grain surface, we found that this time equals to  $1.5 \times 10^3$  year. This time is short enough than the age of NGC2264 IRS1. Thus the accretion of gas-phase species onto grain surfaces and subsequent surface chemistry produce grain mantles rich in saturated species. So our calculation in this model gives only eight species in agreement with observations. This is due to the negligible effect of thermal desorption as seen above in description of table (4).

For our models M3 and M4, we considered NGC2264 IRS1 as a point hot core. Also as Willacy (2007) assumed, the mantle abundances of some species produced from the time-dependent chemistry at 1 Myrs of molecular dense cloud of temperature 10K are used as the initial inputs to M3 and M4, ( see table 5 ).

**Table: 5 Input mantle abundances in our M3 and M4.**

Species	Mantle abundance	Species	Mantle abundance	Species	Mantle abundance
CO	3.5(-6)	CO <sub>2</sub>	3.1(-7)	H <sub>2</sub> CO	4.0(-6)



H <sub>2</sub> O	1.2(-4)	N <sub>2</sub>	7.3(-8)	HCN	4.6(-6)
HC <sub>3</sub> N	3.7(-7)	HNC	7.2(-7)	CH <sub>3</sub> CN	1.5(-8)
NH <sub>3</sub>	1.0(-5)	C <sub>2</sub> H <sub>2</sub>	1.9(-6)	CH <sub>4</sub>	1.4(-6)

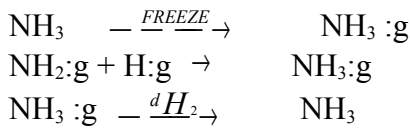
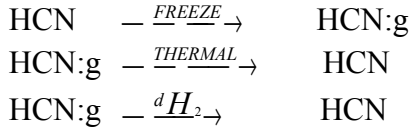
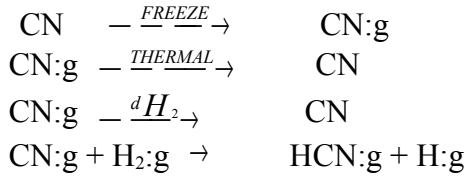
Note that: this values are taken from Willacy (2007)

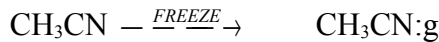
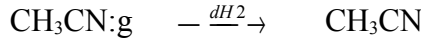
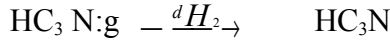
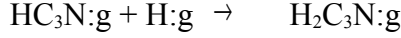
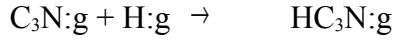
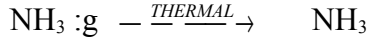
As we see form table (3) the time of thermal evaporation of NGC2264 IRS1 is shorter than that of accretion. Thus our calculated abundances in M3, give us only eleven species are in agreement with observations.

When we change the rate of H<sub>2</sub> formation on grain surface to the value considered in model M4 to fit the observation of H and H<sub>2</sub>, we see that the resulting fractional abundances of all species shown in table (3) are in agreement with observations. In this model the chemical route of formation and destruction of key observed species on grain surface depends on thermal evaporation, freezing on grain surface, grain-grain surface reactions, desorption by H<sub>2</sub> formation (dH<sub>2</sub>) and photo-desorption (pdd). So this model is sensitive to any change for the rate of H<sub>2</sub> formation on grain surface.

In M4 the Nitrogen containing species on the grain surface becomes CN, HCN, HC<sub>3</sub>N, NH<sub>3</sub> and CH<sub>3</sub>CN. The chemical route of these species on and off grain surface are:

For CN

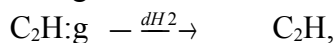
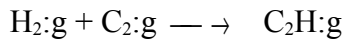
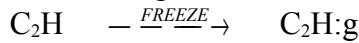


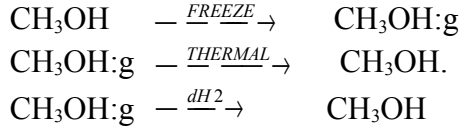
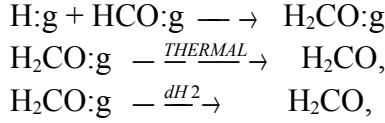


From the last reactions, we see that the freezing on grain surface is one of the main routes of formation of all species, while the thermal desorption is one of the main routes of destruction of CN, HCN and  $\text{NH}_3$ . This is because the evaporation time of these species is small and the critical temperature near the considered one. But the effect of thermal desorption on the destruction of  $\text{HC}_3\text{N}$  and  $\text{CH}_3\text{CN}$  is negligible.

The chemistry of the key observed Nitrogen containing species in gas-phase in this model are : CN molecule is formed from the reaction the cosmic-ray dissociation for  $\text{CH}_3\text{CN}$ .  $\text{CH}_3\text{CN}$  is mainly produced by the radiative association between HCN and  $\text{CH}_3^+$ . Also  $\text{HC}_3\text{N}$  is mainly formed from neutral-neutral reaction of  $\text{C}_2\text{H}_2$  with CN. So the abundances of  $\text{CH}_3\text{CN}$  and  $\text{HC}_3\text{N}$  depends on the abundances of HCN and CN, respectively. While ammonia is formed by dissociative recombination of  $\text{NH}_4^+$  with electron and destroyed by ionized molecule to produce  $\text{NH}_2$ .

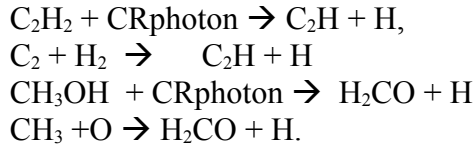
Also the species containing Carbon on grain surface are  $\text{C}_2\text{H}$ ,  $\text{H}_2\text{CO}$  and  $\text{CH}_3\text{OH}$ . The routes of formation and destruction of these species on and off grain surface are



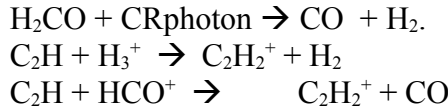


For this group of molecules the grain surface reactions appears only in the formation of  $\text{C}_2\text{H}_2$  and  $\text{H}_2\text{CO}$  on the grain surface.

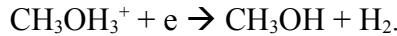
The chemistry of the key observed species Carbon containing species in gas-phase in this model are: The formation of the unsaturated organic species  $\text{C}_2\text{H}$  molecules and the complex organic species  $\text{H}_2\text{CO}$  are,



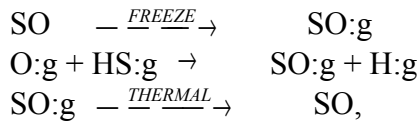
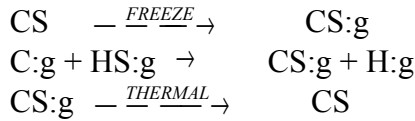
While the destructions are

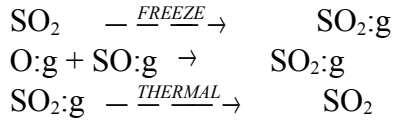


The formation of methanol  $\text{CH}_3\text{OH}$  is



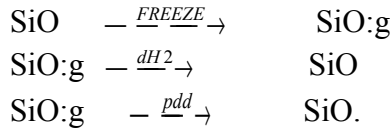
The neutral Sulfure species in our model on grain surface are CS, SO and  $\text{SO}_2$ . The chemical routes of these species are the same as that of Nitrogen and Carbon species, except the destruction by desorption of  $\text{H}_2$  formation ( $\text{dH}_2$ ). The formation and destruction of these species are:





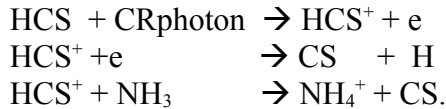
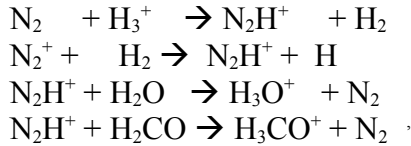
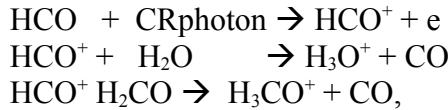
The chemistry of these key observed species of neutral Sulfure are: CS molecule is mainly generated by  $\text{HCS}^+ + e \rightarrow \text{CS} + \text{H}$ . Again CS reacts with  $\text{H}_3^+$  to form  $\text{HCS}^+$  and molecular hydrogen. The main formation of SO depends on the rate of cosmic-ray ionization and the abundance of  $\text{SO}_2$  ( i.e  $\text{SO}_2 + \text{CRphoton} \rightarrow \text{SO} + \text{O}$ ). While  $\text{SO}_2$  is formed by  $\text{SO} + \text{OH} \rightarrow \text{SO}_2 + \text{H}$  and  $\text{HSO}_2^+ + e \rightarrow \text{SO}_2 + \text{H}$ . In our model the relation between SO and CS comes from the reaction  $\text{C} + \text{SO} \rightarrow \text{CS} + \text{O}$ .

In our model M4 Silicon monoxide SiO is formed by freezing on grain surface and destroyed by desorption of  $\text{H}_2$  formation and photo-desorption (pdd), as:



In gas-phase for this model formation of silicon monoxide depends on the oxygen molecule and silicon atoms.

The ionic species  $\text{HCO}^+$ ,  $\text{N}_2\text{H}^+$  and  $\text{HCS}^+$  in our model M4 are formed and destructed by



From the last reactions we find that the dominant chemistry routes of the ionic species in high density and high temperature differ from that of high density and low temperature, as predicted by Amin and El Nawawy (2005). The cosmic ray induced photon is the main route of formation of  $\text{HCO}^+$  and  $\text{HCS}^+$ , while the ion-molecule reaction of  $\text{H}_3^+$  with  $\text{N}_2$  (which has a large abundance due to its formation on grain surface and go out to the gas) and  $\text{N}_2^+$  with  $\text{H}_2$  are the main route of formation of  $\text{N}_2\text{H}^+$ . The water, ammonia and formaldehyde arise as the main species responsible for destruction of  $\text{HCO}^+$ ,  $\text{N}_2\text{H}^+$  and  $\text{HCS}^+$ . The destruction of  $\text{N}_2$  by formaldehyde produce  $\text{N}_2\text{H}^+$  which return to react with  $\text{H}_3^+$  to form  $\text{N}_2$  again. So our model M4 predict high abundance for  $\text{N}_2\text{H}^+$ .

#### 4 Conclusions.

we have investigated the gas-phase and gas-grain chemistry for NGC2246 IRS1 by making use of an extensive chemical network. The gas-phase pseudo time dependent models predict the abundance of some key observed species. Dissociative recombination with electron play the main route of formation for CS,  $\text{NH}_3$ , HCN and  $\text{SO}_2$ , while the reaction with cosmic-ray induced photon play the main route of formation for  $\text{H}_2\text{CO}$ , CN and SO. Also atomic Oxygen plays the main route of formation for  $\text{H}_2\text{CO}$ . For most of the all key observed species cosmic ray and cosmic-ray induced photon play the main route of destruction. Gas phase models fail to predict the abundances of the ionic species in addition to the molecular species  $\text{HC}_3\text{N}$ ,  $\text{C}_2\text{H}$ ,  $\text{CH}_3\text{OH}$  and  $\text{CH}_3\text{CN}$ .

For gas-grain models the thermal desorption, grain surface reactions and the desorption by  $\text{H}_2$  formation and the freezing on grain surface play the main routes of formation and destruction of neutral species. Only for SiO the photo desorption is important in its formation. All of the key observed species in NGC2246 IRS1 predicted by gas-grain chemistry, particularly when we reduced the rate of  $\text{H}_2$  formation on grain surface to  $1.4 \times 10^{-17}$  (or  $T_d \times 3.33 \times 10^{-3}$ )<sup>0.5</sup>.

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