LETTER

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Letter to the Editor

Can DNA bases be produced during molecular cloud collapse?

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Abstract. Using a reasonably large chemical reaction network consisting of 421 species, we show that along with normal chemical evolution of molecular cloud during collapse and star formation, significant amount of adenine, a DNA base, may be produced after an evolution of 10^{6-7} years. This findings may shed light on whether life on earth had to begin from scratch or these molecules could have contaminated the earth from the beginning.

Key words: ISM: molecules – ISM: clouds – stars: formation – molecular processes

1. Introduction

Understanding origin of life on earth is a very challenging astrophysical problem of today. Study of isotopic ratios on carbon inclusions in ferric salt deposits in Greenland shows that life existed on earth before 3.85 billion years (Mojzsis et al. 1996; Holland 1997; Schidlowski 1993) or possibly even before 4 billion years (Mukhin & Gerasimov 1993). On the other hand, data from isotope systematics show that the earth is between 4.55 to 4.57 billion years old (Faure 1986). The time available for life to develop on the earth from scratch is possibly around $0.5-0.6$ billion years which is very short (Crick & Orgel 1973). One of the ways the formation of life on earth could be assisted if the building blocks of life, namely, amino acids and at least some of the bases of DNA could be produced well before the planetary formation, presumably during chemical evolution of molecular clouds. Whereas extensive work is present in the literature to study evolution of some of the organic and inorganic molecules, no work is reported so far which study the formation of bio-molecules or pre-biotic molecules such as amino acids, sugars, DNA, RNA etc.

Bases of DNA such as adenine ($H_5C_5N_5$) can be produced by successive addition of HCN molecules in four steps (Volkenshtein, 1983). In the present *letter* we perform a hydrodynamic simulation and followed chemical evolution during the molecular cloud collapse and show that a significant amount of adenine (with mass fraction $X_{adenine} \sim 10^{-10}$) could be produced. This indicates that planets and comets could have formed with contaminations of pre-biotic molecules. If correct, this may resolve a long-standing problem of origin of lives on earth.

2. Reaction network

We take the UMIST database (Millar, Farquhar & Willacy 1997; hereafter referred to as MFW97) as our basis of chemical reactants and reactions, but added several new reactions such as synthesis of amino acids (alanine and glycine), hydroxy-acids (glycolic and lactic acids), DNA base (adenine, see, Volkenshtein 1983), urea synthesis etc. These new reactions make the total number of species to be 421. The rate co-efficients of these additional reactions are difficult to find, especially in the environs of a molecular cloud. To use UMIST database, the rate constant for a two body reaction is written as (MFW97),

$$k = \alpha(T/300)^{\beta}\exp(-\gamma/T) \ \ \mathrm{cm}^3\ s^{-1} \qquad (1)$$

where, α, β and γ are constants and T is the temperature. Amino acid synthesis rate was estimated from Fig. 8 of Schulte & Shock (1995). Urea synthesis rate is kept comparable to the rates given in UMIST table. The rate constants were taken to be $\alpha = 10^{-10}$, $\beta = \gamma = 0$ for each two-body reactions. The rate constants for adenine synthesis was chosen to be similar to other two body reactions [$\alpha = 10^{-10}$ $\beta = \gamma = 0$ for each HCN addition in the chain $HCN \rightarrow CH(NH)CN \rightarrow NH_2CH(CN)_2 \rightarrow NH_2(CN)C = C(CN)NH_2 \rightarrow H_5C_5N_5$ (adenine)]. This should provide a sufficiently good estimate for the final abundance of these pre-biotic molecules.

Initial composition of the cloud before the simulation begins is kept to be the same as in MFW97, and formation of H_2 is included using the grain-surface reaction with rates as in MFW97. The initial *mass fractions* are taken to be the same as in MFW97 (but converted to mass fractions), i.e., H:He:C:N:O:Na:Mg:Si:P:S:Cl:Fe = 0.64:0.35897:5.6×10^{-4}:1.9×10^{-4}:1.81×10^{-3}:2.96×10^{-8}: 4.63×10^{-8}:5.4×10^{-8}:5.79×10^{-8}:4.12×10^{-7}:9×10^{-8}:1.08×10^{-8}.

3. Hydrodynamic considerations

We use simple molecular cloud model with generic initial conditions: initial size of the molecular cloud $r_0 = 3 \times 10^{18}$cm,

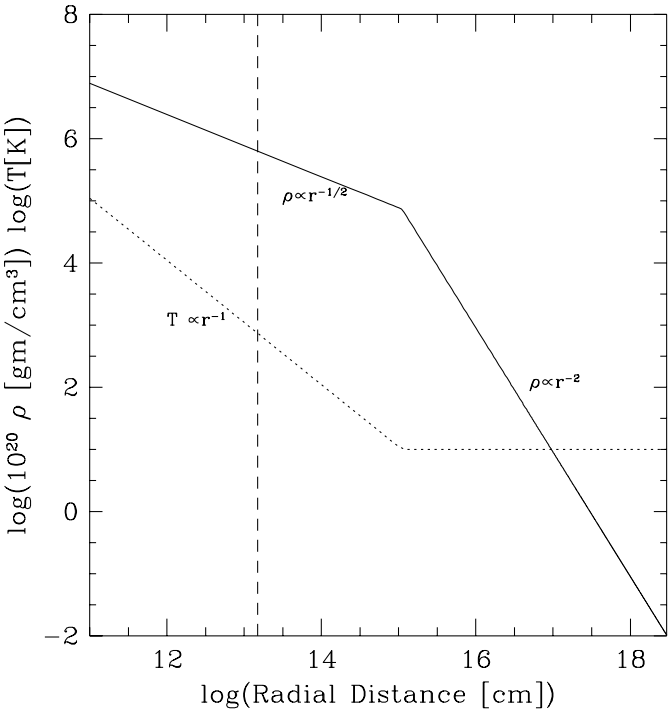

Fig. 1. Log-log plot of temperature (dotted) and mass density (in units of 10^{20}) as functions of the radial distance. Vertical dashed line is drawn at 1AU.

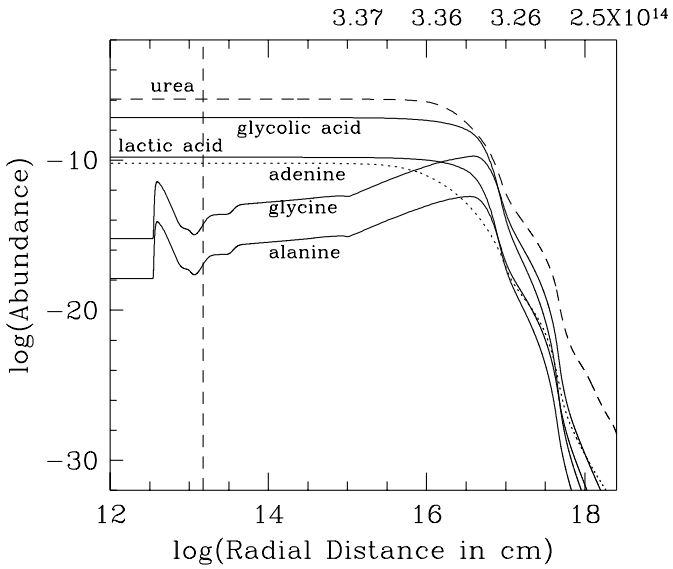

Fig. 2a Log-log plot of the mass fractions of some of the lighter and intermediate mass species as functions of the radial distance. Alternate species have been plotted with dotted curves for clarity. Upper axis shows time elapsed in seconds since collapse began. Vertical dashed line is drawn at 1AU.

average temperature of the cloud $T = 10$K, and angular velocity of the cloud $\Omega = 10^{-16}$ rad s^{-1}. The sound speed becomes $a_s = (kT/\mu m_H)^{1/2} \sim 19200$cm s^{-1} and corresponding initial density (Shu, Adams & Lizano 1987) is $\rho = a_s^2/2\pi G r^2 = 10^{-22}$g cm^{-3} and accretion rate is $\dot{M} = 1.06\times10^{20}$g s^{-1}. Here, $\mu = 2.3$ mean molecular weight, m_H is the mass of the hydrogen atom, and k is the Boltzmann constant. In the isothermal phase of the cloud collapse, density $\rho \propto r^{-2}$ (Chandrasekhar 1939) and the velocity is constant. When opacity becomes high enough to trap radiations (say, at $r = r_{tr}$), the cloud collapses adiabatically with $\rho \propto r^{-3/2}$. In presence of rotation, centrifugal barrier forms at $r = r_c$, where centrifugal force balances gravity. Density falls off as $\rho \propto r^{-1/2}$ in this region (Hartmann, 1998). Following Shu, Adams & Lizano (1987), we compute the density, temperature and velocity distribution inside the cloud and follow the chemical evolution at the same time. With density chosen as above, the initial constant velocity of infall becomes 8900cm s^{-1} and below $r = r_c$ velocity $\propto r^{-1/2}$ to preserve the accretion rate in a disk like structure of constant height. Since for the parameters chosen (generic as they are) $r_c > r_{tr}$, we chose $T \propto 1/r$ inside the centrifugal barrier ($r < r_c$) as in an adiabatic flow. We follow the collapse till a radius of 10^{12}cm is reached. Fig. 1 shows the temperature and mass density (in units of 10^{20}) distribution in a log-log scale. Our choice of Ω is small by at least an order of magnitude from that of the observed value in some of the clouds. This was done to obtain atmosphere at a distance of around 1AU from the proto-star to be as close to reducing ($C/O > 1$).

4. Results

Fig. 2a shows the log-log variation of mass fractions of some of the light and intermediate species of our simulation with radial distance (in cm). For clarity, we plot the curves alternately by solid and dotted type. In Fig. 2b, we plot the variation of more complex molecules. Since they start with zero abundances, we plot them from radius 2.5×10^{18}cm for clarity. We put a long dashed vertical line at 1AU, the distance of the earth with respect to the sun. On the upper axis, we have put time (in seconds) elapsed since the beginning of collapse at radial distances of 10^{18}cm, 10^{17}cm, 10^{16}cm and 10^{15}cm respectively. Towards the end of the collapse, time spent is negligible.

Because of low initial velocity, H, N, C and O are depleted much before 100AU and HCN, NH_3, CH_3CN etc. rises as also the more complex molecules (Fig. 2b) which form out of them. Inside r_c, as matter falls faster and spends lesser time, the depletion of lighter molecules are controlled, until the density and temperature also rises so high that depletion started once more. Inside, 3×10^{12} cm, the composition changes in a very short timescale Around $r \sim 10$AU, the mass fractions of adenine, urea and glycine are already significant. At $r = 1$AU, $X_{adenine} = 6 \times 10^{-11}$. Since the mass of the earth is around 4×10^{27}g, this corresponds to 2.4×10^{17}g of adenine which could have contaminated the earth at the time of formation (it could be higher since metallic content of earth is much above the average molecular value. Also, one has to include the effect of dust-gas mixture in the molecular cloud) This computation, does not consider the destructions of adenine at a higher temperature region, and it is likely that much of these contaminants are destroyed during collapse and formation of proto-earth. However, comets formed in the inner cloud could carry away these

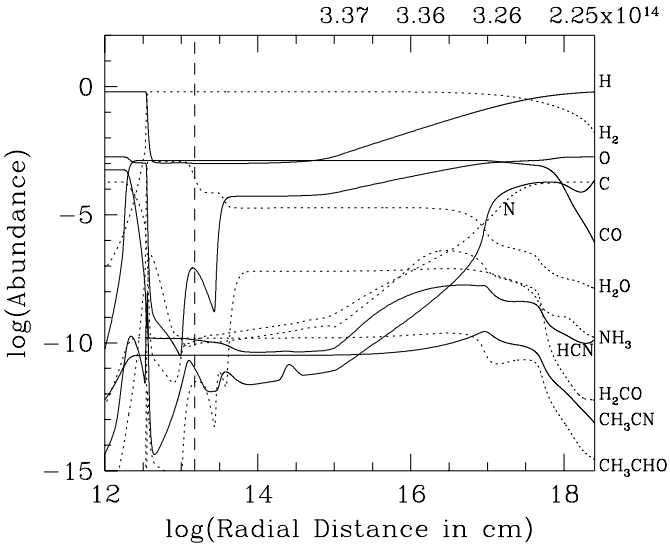

Fig. 2b Log-log plot of the mass fractions of a few complex molecules (marked) as functions of the radial distance. Upper axis shows time elapsed in seconds since collapse began. Vertical dashed line is drawn at 1AU.

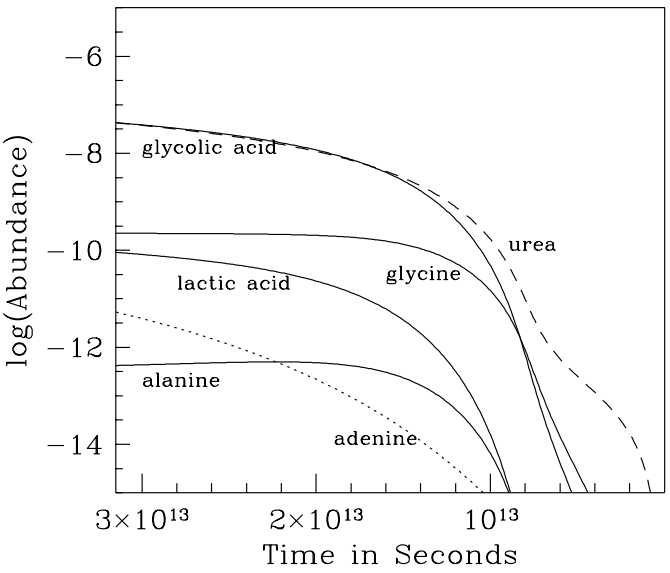

Fig. 3. Log-log plot of the mass fractions of some pre-biotic molecules (marked) as functions of time during the evolution of a static cloud of constant density and temperature for 10^6 years.

pre-biotic molecules and deposit them during future impacts on planets. It is to be noted that around 1AU, the composition is close to reducing ($C/O > 1$) type (Fig. 2a) which is favourable for the formation of bio-molecules.

Since regions of low density of molecular cloud could have a very long evolution time scale, it may of interest whether pre-biotic molecules could have formed in a very low density isothermal region. To this effect, we choose a cloud of mass density $\rho = 1.6 \times 10^{-19}$g cm^{-3} and $T = 10$K and let it evolve for 10^6 years. Fig. 3 shows the results of this simulation where we plot the variation of abundance with time (in seconds). We find that the abundance of adenine, for instance, is around 5×10^{-12}. This is a very generic condition, and the abundance is significant. We therefore believe that adenine could be produced during the molecular cloud collapse.

5. Concluding remarks

It is generally thought that molecules vital to living systems on earth may have started from scratch. In this *Letter*, we have explored the possibility of formation of a DNA base, namely adenine, and a few of the simpler amino acids during a generic molecular cloud collapse and show that mass fraction of adenine is significant which might have contaminated the planetary disk even before the formation of the planets themselves. In a static evolution of a cloud of constant density and temperature, the formation of adenine is also important, and therefore our conclusion may be very generic. The rates we have chosen are reasonable, though uncertainties of an order of magnitude cannot be ruled out at this stage as more accurate estimates require one to have temperature dependent rate coefficients of both forward and reverse reactions.

Since earth is a generic planet and since it seems apparent that bio-molecules are as naturally produced as any other complex molecules, we believe that DNA bases produced in collapsing cloud could have contaminated the earth, and at the same time there should be many such planets in each galaxy where DNA based lives should flourish. It is not yet clear whether or not these molecules survived during further evolution of planetary disks leading to eventual formation of planets or actual contaminations were made much later by comets carrying away protecting these molecules. These vital issues will be addressed in due course.

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