Molecular Evolution in Interstellar Clouds. I

---Ion Chemistry in Dense Clouds---

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Molecular abundances are calculated time-dependently using a chemical scheme which is constructed to represent the evolutional feature of all molecules containing up to 2 heavy atoms (C, N, O, S, and Si) and consisted of the surface recombination of hydrogen on grains and 2884 gas phase reactions of 234 species. For the model adopted ($n_H=10^5 \text{ cm}^{-3}$, $T=30 \text{ K}$, $\zeta_H=10^{-10} \text{ s}^{-1}$ per H atom), observed molecules are produced successfully and attain their steady-state abundances at $t=\sim 2 \times 10^{16} \text{ s}$, which is longer than the evolutional time scale of dense clouds. Molecules containing carbon (except carbon in C-O bond) have peak abundances at $t=\sim 10^{10} \text{ s}$, when most C atoms are consumed in forming CO molecules. The C/CO ratio is a good indicator of molecular evolution in dense clouds.

§ 1. Introduction

The formation of interstellar molecules has been discussed, in most cases, under either of the two extreme astronomical conditions, diffuse or dense clouds. The mechanism of molecular formation in diffuse, optically thin clouds is fairly well established—the observational abundances are in the error of estimates, though some problems such as CH⁺ deficiency still remain unresolved. On the other hand, the theory is still qualitative on molecular formation in dense clouds, where large complex molecules as well as ions and radicals are discovered by radio and microwave observations. The synthesis of complex molecules by recombination of radicals on grain surfaces was proposed by Iguchi and developed by Allen and Robinson, but they adopted several assumptions on elementary processes which have not yet been confirmed by experiment.

The gas-phase models involved mainly ion-neutral reactions following the cosmic-ray ionizations. The reaction schemes were discussed by Harteeck and Reeves, Watson, Herbst and Klempner, and Mitchell, Ginsburg and Kuntz. Iglesias extended the model of Herbst and Klempner and calculated molecular abundances time-dependently including the charge transfer reactions of molecular ions with metal atoms, whose importance had been pointed out by Oppenheimer and Dalgarno. However, the number of reactions in their chemical models was limited and many important ion-neutral collisions were not taken into account.

On the other hand, it has been clarified by the investigations of time-dependant models of molecular formation that the time for major neutrals to reach their steady state is comparable with the evolutional time scale of clouds ($10^{13}$ to $10^{15}$ s).
It is long enough for heavier molecules to be produced to substantial amount, because most ion-neutral reactions have rate coefficients of magnitude of Langevin rates, \( k_L = \sim 10^{-9} \text{cm}^3 \text{s}^{-1} \). Thus, many species are coupled tightly with one another by numerous reactions, only a part of which is investigated by experiment.

In this paper, a chemical scheme is carefully constructed to represent the molecular evolution in dense clouds. All ion-neutral reactions of species containing up to 2 heavy atoms (C, N, O, S and Si) are surveyed. For most ion-neutral collisions, the reaction rate coefficients (though they should not much differ from \( k_L \)) are not known, much less what kind of products should be yielded. We choose suitable reaction channels from many exothermic exits of products. Including of condensation reactions of species containing up to 2 heavy atoms requires that species containing up to 4 heavy atoms should be taken into account. As a result, 234 species are treated and 2885 reactions are included in our chemical scheme (§ 2).

A model calculation using this reaction network is carried out time-dependently with fixed density and temperature. It is assumed that all elements (H, C, N, O, S, Si and Mg) are locked up in atomic form at the initial stage of calculation. The Mg atom is included as the representative of metals, because the cosmic abundance of Mg is the highest among metals. UV radiation is neglected because the molecular evolution takes place when clouds become optically thick for UV radiation. The investigations of molecular formation in clouds of intermediate stage of evolution (optically thin to thick) show that the composition of molecules when clouds become optically thick is not atomic, of course, but a function of time scale of contraction and the mass of the clouds. Since the main purpose of this work is to construct a chemical scheme of molecular formation in the gas phase, the effects of initial abundances are not considered. Model calculations of chemical evolution starting from atomic species will exhibit most clearly the mechanism of molecular formation. The effects of variation of initial abundances and physical condition will be discussed elsewhere.

§ 2. Chemical reaction schemes

2.1. Ionization by cosmic rays and \( H_2 \) formation on grain surfaces

In dense clouds, it is convinced that the hydrogen is mostly in the form of \( H_2 \) molecule. However, very few gas-phase processes produce \( H_2 \) molecules, while the recombination of H atoms on grain surfaces is the most established surface reaction and explains well the observations. Because radiative association reactions between atoms are very slow (\( 10^{-17} \) to \( 10^{-19} \text{cm}^3 \text{s}^{-1} \)) and heavier atoms are much less abundant than H atom, this surface recombination must be the first and the most effective bond formation process in dense clouds. The ion-neutral reactions involving \( H_2 \) then form heavier molecules successively.

The external ionization source for dense clouds is high-energy cosmic rays.
Table I. Effective reactions in dense clouds.

Only 448 effective reactions are tabulated (see § 3).

References: CD78, H77, F76, F73, FLM77, SA78, SA77, JB74, RLA73, LBJ73A, G78, LBJ73C, MM79, MM79B.

(a) Grain surface reactions.

The number density of grains relative to \( n_H \) is taken to be \( 10^{-11} \), and the radius of grains to be 0.034\( \mu \). Recombination efficiency is assumed to be unity.

<table>
<thead>
<tr>
<th>No.</th>
<th>Reactions</th>
<th>Rates per H atom (s(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( H + H \rightarrow H_2 )</td>
<td>( 2.7 \times 10^{-18} \sqrt{T_{n_H}} )</td>
</tr>
</tbody>
</table>

(b) Ionization and dissociation reactions by cosmic rays.

The ionization rate of an H atom including the effects of secondary electrons, \( \zeta_n \), is taken to be \( 10^{-18} \) s\(^{-1}\).

<table>
<thead>
<tr>
<th>No.</th>
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<th>Rates (s(^{-1}))</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>( H_2 \rightarrow H^+ + H + e )</td>
<td>( 5.3 \times 10^{-20} )</td>
<td>CD78</td>
</tr>
<tr>
<td>4</td>
<td>( \rightarrow H^+ + e )</td>
<td>( 1.8 \times 10^{-18} )</td>
<td>CD78</td>
</tr>
<tr>
<td>5</td>
<td>( \rightarrow H + H )</td>
<td>( 4.4 \times 10^{-18} )</td>
<td>CD78</td>
</tr>
<tr>
<td>6</td>
<td>( He \rightarrow He^+ + e )</td>
<td>( 1.1 \times 10^{-18} )</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>( N \rightarrow N^+ + e )</td>
<td>( 4.4 \times 10^{-18} )</td>
<td></td>
</tr>
</tbody>
</table>

Most of the primary ions, \( H_2^+ \) and \( He^+ \), are converted to other ions by ion-neutral reactions before they recombine with electrons. The formation rates of ions other than \( H_2^+ \) and \( He^+ \) by these processes are usually larger than those due to direct ionization by cosmic rays by a factor of \( 10^4 \) to \( 10^8 \). Therefore, the direct ionizations (including ionizations by secondary electrons) are included only for several major components in dense clouds.

The surface reaction and reactions by cosmic-ray bombardment are summarized in Tables I (a) and (b).

2.2. Ion-neutral reactions and the selection of species in the chemical scheme

Since radicals and ions are stable because of the low density and the low temperature, there should be many kinds of ionic and neutral species in dense clouds. They form a huge network of possible ion-neutral reactions whose rate coefficients are of the same order of magnitude, \( k_L = \sim 10^{-9} \text{cm}^3\text{s}^{-1} \). Besides, the time for clouds evolution is so long (not less than the free fall time, \( \tau_f = 10^{15.5} \sqrt{n_H} \text{s} \), where \( n_H \) is the number density of hydrogen, \( n(H) + 2n(H_2) \)) that even very infrequent reactions, such as reactions of species which are not abundant, could affect the final abundances of more abundant species. Thus, numerous reactions are coupled closely with one another, and it is very difficult to simplify the mechanism of molecular evolution.

We intend to clarify the formation and destruction of molecules containing
up to 2 heavy atoms (C, N, O, S and Si). For this purpose, all the collisions of their ions and neutrals are considered. The ions which react with H\textsubscript{2} at the Langevin rate are excluded from this consideration because they are less abundant than their daughter ions by at least a factor of \(~x(H\textsubscript{2}) \times 10^3\), where \(x(X)\) is the abundance of \(X\) relative to hydrogen. Some near-saturated and saturated molecules, such as C\textsubscript{2}H\textsubscript{5} and C\textsubscript{6}H\textsubscript{6}, and their ions are also excluded since we have estimated that they do not become very abundant. Thus, 28 ions and 45 neutrals are chosen which hereafter we call class I species. The exothermic exits of all ion-neutral collisions of class I species are searched. As the products, we consider 164 ions and 150 neutrals including class I species, whose heats of formation were taken from Wagman et al.,\textsuperscript{12} Franklin et al.,\textsuperscript{13} Darwent,\textsuperscript{10} the JANAF Thermochemical Tables,\textsuperscript{10} Franklin,\textsuperscript{15} Rosenstock et al.,\textsuperscript{17} Bohme,\textsuperscript{18} McAllister\textsuperscript{19} and Allen and Robinson.\textsuperscript{20} Generally, an ion-neutral collision has many exothermic channels. For example, the C\textsubscript{2}H\textsubscript{2} + HCO reaction has 12 exothermic exits. We select a set of reactions from these exothermic channels on the basis of the existing experimental data, especially those of Huntress\textsuperscript{20} who summarized experimental results of his group and discussed the quantitative aspects of ion-neutral reactions. The reactions chosen include condensation reaction, proton transfer, charge transfer, H or H\textsuperscript{-} abstraction and exchange reaction. The reaction rate coefficients are taken to be Langevin, and the branching ratios are assumed to be even for all possible channels when no experimental data are available.

These reactions produce species other than those of class I. All the combinations of these product ions and neutrals are not considered. Since they involve up to 4 heavy atoms, it is necessary to treat heavier molecules including 5 to 8 heavy atoms for complete tracing of them, which is practically impossible. Only proton transfer, charge transfer with major components, H abstraction reactions with H\textsubscript{2} molecule and the dissociative recombination with electrons are searched. Here, the major components, H\textsuperscript{+}, H\textsubscript{3}\textsuperscript{+}, CH\textsubscript{3}\textsuperscript{+}, H\textsubscript{2}O\textsuperscript{+}, S\textsuperscript{+}, Si\textsuperscript{+}, Mg\textsuperscript{+}, HCNH\textsuperscript{+}, HCO\textsuperscript{+}, C\textsubscript{2}H\textsuperscript{+}, H, H\textsubscript{2}, C, N, O, S, Si, Mg, H\textsubscript{2}O, CO, N\textsubscript{2}, NO and O\textsubscript{2}, are chosen from the consideration of the flow of elements in dense clouds. The new species produced by these reactions are also treated as noted above. After repeating these procedures several times, no new species are produced any more.

After all, 100 ions and 60 neutrals, which hereafter we call class II species, are added to the class I species. The total number of ion-neutral reactions in the scheme is now 2301, a part of which is tabulated in Table I(c) (for the selection, see § 3).
Table I (c) Ion-neutral reactions.

Rate coefficients without references are taken to be those of the Langevin with equal branching ratios.

<table>
<thead>
<tr>
<th>No.</th>
<th>Reactions</th>
<th>Rate coef. (cm$^{-1}$s$^{-1}$)</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>$H^+ + H_2O \rightarrow H_2O^+ + H$</td>
<td>$8.2 \times 10^{-4}$</td>
<td>H77</td>
</tr>
<tr>
<td>41</td>
<td>$+ CH_2NH_2 \rightarrow CH_2NH_2^+ + H$</td>
<td>$5.2 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>46</td>
<td>$+ CS \rightarrow CS^+ + H$</td>
<td>$5.3 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>56</td>
<td>$+ SN \rightarrow NS^+ + H$</td>
<td>$5.3 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>57</td>
<td>$+ O_2 \rightarrow O_2^+ + H$</td>
<td>$1.2 \times 10^{-4}$</td>
<td>H77</td>
</tr>
<tr>
<td>59</td>
<td>$+ H_2O \rightarrow H_2O^+ + H$</td>
<td>$3.6 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>$+ SO \rightarrow SO^+ + H$</td>
<td>$3.7 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>61</td>
<td>$+ SiO \rightarrow SiO^+ + H$</td>
<td>$4.1 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>74</td>
<td>$+ C_2 \rightarrow C_2^+ + H$</td>
<td>$4.4 \times 10^{-3}$</td>
<td></td>
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<tr>
<td>80</td>
<td>$+ CHCHO \rightarrow CHCHO^+ + H$</td>
<td>$5.1 \times 10^{-3}$</td>
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<tr>
<td>82</td>
<td>$+ HNCO \rightarrow HNCO^+ + H$</td>
<td>$4.2 \times 10^{-3}$</td>
<td></td>
</tr>
<tr>
<td>83</td>
<td>$+ HCONH_2 \rightarrow HCONH_2^+ + H$</td>
<td>$4.8 \times 10^{-3}$</td>
<td></td>
</tr>
<tr>
<td>85</td>
<td>$+ HNC \rightarrow HNC^+ + H$</td>
<td>$5.3 \times 10^{-3}$</td>
<td></td>
</tr>
<tr>
<td>87</td>
<td>$+ OCS \rightarrow OCS^+ + H$</td>
<td>$6.7 \times 10^{-3}$</td>
<td></td>
</tr>
<tr>
<td>90</td>
<td>$+ CS_2 \rightarrow CS_2^+ + H$</td>
<td>$7.0 \times 10^{-3}$</td>
<td></td>
</tr>
<tr>
<td>93</td>
<td>$+ C_4 \rightarrow C_4^+ + H$</td>
<td>$5.3 \times 10^{-4}$</td>
<td></td>
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<tr>
<td>101</td>
<td>$+ C_3H_2CN \rightarrow C_3H_2CN^+ + H$</td>
<td>$5.9 \times 10^{-4}$</td>
<td></td>
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<tr>
<td>102</td>
<td>$+ C_3H_2CHO \rightarrow C_3H_2CHO^+ + H$</td>
<td>$5.3 \times 10^{-4}$</td>
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<tr>
<td>105</td>
<td>$H_2^+ + H_2 \rightarrow H_2^+ + H$</td>
<td>$2.1 \times 10^{-4}$</td>
<td>H77</td>
</tr>
<tr>
<td>180</td>
<td>$H_2^+ + C \rightarrow CH^+ + H_2$</td>
<td>$1.5 \times 10^{-9}$</td>
<td></td>
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<tr>
<td>181</td>
<td>$+ O \rightarrow OH^+ + H_2$</td>
<td>$8.0 \times 10^{-10}$</td>
<td>F76</td>
</tr>
<tr>
<td>182</td>
<td>$+ S \rightarrow SH^+ + H_2$</td>
<td>$1.9 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>183</td>
<td>$+ Si \rightarrow SiH^+ + H_2$</td>
<td>$2.5 \times 10^{-3}$</td>
<td></td>
</tr>
<tr>
<td>184</td>
<td>$+ CH \rightarrow CH^+ + H_2$</td>
<td>$1.8 \times 10^{-3}$</td>
<td></td>
</tr>
<tr>
<td>185</td>
<td>$+ CH_2 \rightarrow CH_2^+ + H_2$</td>
<td>$2.0 \times 10^{-9}$</td>
<td></td>
</tr>
<tr>
<td>186</td>
<td>$+ CH_3 \rightarrow CH_3^+ + H_2$</td>
<td>$2.2 \times 10^{-9}$</td>
<td></td>
</tr>
<tr>
<td>187</td>
<td>$+ CH_4 \rightarrow CH_4^+ + H_2$</td>
<td>$2.4 \times 10^{-9}$</td>
<td>H77</td>
</tr>
<tr>
<td>188</td>
<td>$+ NH \rightarrow NH^+ + H_2$</td>
<td>$1.6 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>189</td>
<td>$+ NH_2 \rightarrow NH_2^+ + H_2$</td>
<td>$1.9 \times 10^{-4}$</td>
<td></td>
</tr>
<tr>
<td>190</td>
<td>$+ NH_3 \rightarrow NH_3^+ + H_2$</td>
<td>$4.7 \times 10^{-8}$</td>
<td>H77</td>
</tr>
<tr>
<td>191</td>
<td>$+ OH \rightarrow HO^+ + H_2$</td>
<td>$1.5 \times 10^{-8}$</td>
<td></td>
</tr>
<tr>
<td>192</td>
<td>$+ H_2O \rightarrow H_2O^+ + H_2$</td>
<td>$5.9 \times 10^{-8}$</td>
<td>H77</td>
</tr>
<tr>
<td>193</td>
<td>$+ HS \rightarrow HS^+ + H_2$</td>
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<td></td>
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<tr>
<td>194</td>
<td>$+ H_2S \rightarrow H_2S^+ + H_2$</td>
<td>$3.7 \times 10^{-9}$</td>
<td>H77</td>
</tr>
<tr>
<td>195</td>
<td>$+ SiH \rightarrow SiH^+ + H_2$</td>
<td>$2.5 \times 10^{-8}$</td>
<td></td>
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<tr>
<td>196</td>
<td>$+ C_4 \rightarrow C_4^+ + H_2$</td>
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<td>197</td>
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<tr>
<td>198</td>
<td>$+ C_4H_2 \rightarrow C_4H_2^+ + H_2$</td>
<td>$3.5 \times 10^{-9}$</td>
<td>H77</td>
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<tr>
<td>200</td>
<td>$+ C_4H_3 \rightarrow C_4H_3^+ + H_2$</td>
<td>$1.4 \times 10^{-9}$</td>
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<tr>
<td>201</td>
<td>$+ C_4H_4 \rightarrow C_4H_4^+ + H_2$</td>
<td>$2.2 \times 10^{-8}$</td>
<td>H77</td>
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<tr>
<td>204</td>
<td>$+ C_4H_5 \rightarrow C_4H_5^+ + H_2$</td>
<td>$1.5 \times 10^{-8}$</td>
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<tr>
<td>No.</td>
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<td>-----------</td>
<td>---------------------</td>
<td>------------</td>
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<tr>
<td>205</td>
<td>H₃⁺ + C₂H₄ → C₂H₅⁺ + H₂ + H₂</td>
<td>3.4 × 10⁻⁸</td>
<td>H77</td>
</tr>
<tr>
<td>206</td>
<td>H₂CN → HCN⁺ + H₂</td>
<td>2.0 × 10⁻⁸</td>
<td></td>
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<tr>
<td>207</td>
<td>HCN → HCNH⁺ + H₂</td>
<td>8.0 × 10⁻⁹</td>
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<td>208</td>
<td>HNC → HCNH⁺ + H₂</td>
<td>2.3 × 10⁻⁸</td>
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<tr>
<td>209</td>
<td>H₂CNH → CH₃NH⁺ + H₂</td>
<td>2.5 × 10⁻⁸</td>
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<tr>
<td>210</td>
<td>CO → HCO⁺ + H₂</td>
<td>1.7 × 10⁻⁸</td>
<td>H77</td>
</tr>
<tr>
<td>211</td>
<td>HCO → H₂CO⁺ + H₂</td>
<td>2.2 × 10⁻⁸</td>
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<tr>
<td>212</td>
<td>H₂CO → CH₂OH⁺ + H₂</td>
<td>2.4 × 10⁻⁹</td>
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<tr>
<td>213</td>
<td>+CH₅OH → CH₃OH⁺ + H₂</td>
<td>2.5 × 10⁻⁹</td>
<td></td>
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<tr>
<td>214</td>
<td>+CH₄O → CH₃OH⁺ + H₂</td>
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<td>+CH₄OH → CH₂OH⁺ + H₂</td>
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<td></td>
</tr>
<tr>
<td>216</td>
<td>+CS → HCS⁺ + H₂</td>
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<td></td>
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<tr>
<td>217</td>
<td>+H₂CS → CH₂Si⁺ + H₂</td>
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</tr>
<tr>
<td>218</td>
<td>+N₂ → N₂H⁺ + H₂</td>
<td>1.7 × 10⁻⁹</td>
<td>H77</td>
</tr>
<tr>
<td>219</td>
<td>+NO → HNO⁺ + H₂</td>
<td>1.4 × 10⁻⁹</td>
<td>F73</td>
</tr>
<tr>
<td>220</td>
<td>+O₂ → H₂O⁺ + H₂</td>
<td>6.4 × 10⁻¹⁶</td>
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<tr>
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<td>+H₂ → H₂O⁺ + H₂</td>
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</tr>
<tr>
<td>222</td>
<td>+He → He⁺</td>
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<tr>
<td>223</td>
<td>+C₄ → C₄⁺ + H₂</td>
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<tr>
<td>226</td>
<td>+C₃H → C₃H⁺ + H₂</td>
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<td></td>
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<tr>
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<td>+CH₃CH → CH₃CH⁺ + H₂</td>
<td>3.3 × 10⁻⁹</td>
<td></td>
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<tr>
<td>228</td>
<td>+CH₃CH → CH₃CH⁺ + H₂</td>
<td>3.3 × 10⁻⁹</td>
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<tr>
<td>229</td>
<td>+CH₃CH₂ → CH₃CH₂⁺ + H₂</td>
<td>3.4 × 10⁻⁹</td>
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<tr>
<td>230</td>
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<td>3.4 × 10⁻⁹</td>
<td></td>
</tr>
<tr>
<td>231</td>
<td>+CH₃CH₂ → CH₃CH₂⁺ + H₂</td>
<td>3.4 × 10⁻⁹</td>
<td></td>
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<td>232</td>
<td>+CH₃CH₂ → CH₃CH₂⁺ + H₂</td>
<td>3.4 × 10⁻⁹</td>
<td></td>
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<tr>
<td>233</td>
<td>+CH₃CN → CH₃CN⁺ + H₂</td>
<td>2.8 × 10⁻⁹</td>
<td></td>
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<td>234</td>
<td>+CH₃CN → CH₃CN⁺ + H₂</td>
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<td>+H₂CCO → CH₂CO⁺ + H₂</td>
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<td>+CN → CH⁻ + H₂</td>
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<td>+CH₃N → CH₃N⁺ + H₂</td>
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### Table: Reactions in Interstellar Clouds

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<td>( \text{NH}_3^+ + \text{O} \rightarrow \text{HNO}^+ + \text{H}_2 )</td>
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<td>+ Mg \rightarrow \text{Mg}^* + \text{NH}_3</td>
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<td>O(^+) + H(_2) \rightarrow \text{OH}^+ + H</td>
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<td>CN⁺ + H₂ → HCN⁺ + H</td>
<td>1.2 × 10⁻⁹</td>
<td>H77</td>
</tr>
<tr>
<td>1324</td>
<td>HCN⁺ + H₂ → HCNH⁺ + H</td>
<td>9.0 × 10⁻¹⁰</td>
<td>H77</td>
</tr>
<tr>
<td>1356</td>
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<td>1.0 × 10⁻⁹</td>
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<tr>
<td>1357</td>
<td>+ C₂H → C₂H₂CN⁺ + H</td>
<td>1.1 × 10⁻⁹</td>
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<tr>
<td>1407</td>
<td>H₂CN⁺ + N → CH₂N⁺ + H</td>
<td>6.6 × 10⁻¹⁰</td>
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<td>1408</td>
<td>+ O → OH⁺ + HCN</td>
<td>5.6 × 10⁻¹⁰</td>
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<td>1431</td>
<td>+ C₂ → C₂N⁺ + H₂</td>
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<tr>
<td>1462</td>
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<tr>
<td>1477</td>
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<tr>
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<tr>
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<tr>
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<td>+ N → HCO⁺ + NH</td>
<td>3.3 × 10⁻¹⁰</td>
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<tr>
<td>1557</td>
<td>→ HNCO⁺ + H</td>
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<tr>
<td>1559</td>
<td>+ O → CO₂⁺ + H₂</td>
<td>1.9 × 10⁻¹⁰</td>
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<tr>
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<td>1.8 × 10⁻⁹</td>
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<tr>
<td>1578</td>
<td>+ CH₃ → CH₂CHCHO⁺ + H</td>
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<tr>
<td>1580</td>
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<td>1586</td>
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<td>1660</td>
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<td>1665</td>
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<td>No.</td>
<td>Reactions</td>
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<td>1666</td>
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<td>1673</td>
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<td>1676</td>
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<td>2124</td>
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<td>2129</td>
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<td>2132</td>
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<td>2133</td>
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<td>2159</td>
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<td>2174</td>
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<td>2184</td>
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</table>
2.3. \textit{He}^+ reactions

Since the ionization energy of He is very high, \textit{He}^+ transfers the charge to molecules dissociatively. For class I species, some suitable product channels are chosen and included in the scheme. Heavier molecules (class II) have more exits of products. For example, the \textit{He}^++CH\textsubscript{3}CN reaction has 22 exothermic dissociative charge transfer channels even if we exclude the channels in which the ion has a lighter mass than the neutral fragments. Fortunately, however, the abundance
of He\(^+\) is so small in dense clouds that most neutrals react with other ions before they react with He\(^+\). Only for non-reactive neutral species in class II, the He\(^+\) reactions are included.

Charge transfer reactions between He\(^+\) and heavy molecules such as C\(_2\)H\(_2\) and C\(_2\)H\(_4\) have been observed in the laboratory. However, we neglect reactions of this type except those observed, because most molecules undergo charge transfer reactions with other ions, such as H\(^+\) and C\(^+\), faster than with He\(^+\). The role of He\(^+\) reactions is to decompose the molecules and make the molecular evolution slower.

Table I. (d) He\(^+\) reactions.

Rate coefficients without references are taken to be those of the Langevin with equal branching ratios.

<table>
<thead>
<tr>
<th>No.</th>
<th>Reactions</th>
<th>Rate coef. (cm(^3)s(^{-1}))</th>
<th>References</th>
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<tr>
<td>2313</td>
<td>He(^+)+H(_2)→H(_2^+)+He+H</td>
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<tr>
<td>2329</td>
<td>+OH→O(^+)+He+H</td>
<td>1.3×10(^{-8})</td>
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<td>2341</td>
<td>+C(_2)H→C(_2^+)+He+H</td>
<td>2.1×10(^{-4})</td>
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<tr>
<td>2364</td>
<td>+CN→N(^+)+He+C</td>
<td>8.9×10(^{-14})</td>
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</tr>
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<td>2366</td>
<td>+HCN→CN(^+)+He+H</td>
<td>1.6×10(^{-4})</td>
<td>H77</td>
</tr>
<tr>
<td>2374</td>
<td>+CO→C(^+)+He+O</td>
<td>1.6×10(^{-4})</td>
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<td>2380</td>
<td>+CS→S(^+)+He+C</td>
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<td>+SiC→Si(^+)+He+C</td>
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<td>+N(_2)→N(_2^+)+He</td>
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<td>2417</td>
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<td>+CNN→N(_2^+)+He+C</td>
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<td>→CS(^+)+He+O</td>
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<td>2482</td>
<td>+HCCC→C(_4^+)+He+H</td>
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</table>

2.4. Recombination reactions with electrons

The dissociative recombination reactions have been studied in the laboratory, but the relative amounts of the neutral products have not yet been determined to our knowledge. Theoretical calculations of branching ratios have recently been
carry out by Herbst.\textsuperscript{43} The results are highly dependent on parameters. Another problem arises for dissociative recombination of very heavy molecules, that the kinds of products are numerous. For example, the $\text{C}_4\text{H}_6^+ + e$ reaction has 33 exits of dissociative recombination. Distinct from the $\text{He}^+$ reactions, the dissociative recombination reactions are competitive with ion-neutral reactions for a molecular ion. Especially, they destruct heavy atom-heavy atom bonds, while ion-neutral reactions scarcely do. These effects should not be neglected in considering the molecular evolution.

We include dissociative recombination reactions for all ions except class II ions that react with $\text{H}_2$. We choose suitable, natural products from many exothermic decomposition channels and assume the equal branching ratios. The total rate coefficients are assumed to be $(1-2t) \times 10^{-7} \sqrt{300/T}$ for reactions which have no experimental values. This is not satisfactory, but is the best we can do now.

A part of the included ion-electron recombination reactions is tabulated in Table I (e).

**Table I.** (e) Associative and dissociative recombination reactions.

The rate coefficients without references are taken to be $(1-2t) \times 10^{-7} \sqrt{300/T}$ with equal branching ratios. The temperature is 30K.

<table>
<thead>
<tr>
<th>No.</th>
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<th>References/Notes</th>
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Molecular Evolution in Interstellar Clouds. I

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<tr>
<td>2860</td>
<td>$\rightarrow$ C$_4$H$_8$ + H</td>
<td>6.0 x 10$^{-7}$</td>
<td></td>
</tr>
<tr>
<td>2861</td>
<td>C$_4$H$_3$CN$^+$ + e $\rightarrow$ CCN + CH$_4$</td>
<td>1.6 x 10$^{-8}$</td>
<td></td>
</tr>
<tr>
<td>2862</td>
<td>$\rightarrow$ C$_3$N + H$_2$</td>
<td>1.6 x 10$^{-8}$</td>
<td></td>
</tr>
<tr>
<td>2863</td>
<td>$\rightarrow$ HCCCN + H</td>
<td>1.6 x 10$^{-8}$</td>
<td></td>
</tr>
<tr>
<td>2864</td>
<td>CH$_3$CHCN$^+$ + e $\rightarrow$ CCN + CH$_4$ + H</td>
<td>5.7 x 10$^{-4}$</td>
<td></td>
</tr>
<tr>
<td>2865</td>
<td>C$_4$H$_3$CN$^+$ + e $\rightarrow$ CH$_3$CHCN + H</td>
<td>1.1 x 10$^{-4}$</td>
<td></td>
</tr>
<tr>
<td>2866</td>
<td>C$_3$H$_3$CN$^+$ + e $\rightarrow$ CH$_3$CN + C + H$_2$ + H</td>
<td>3.3 x 10$^{-4}$</td>
<td></td>
</tr>
<tr>
<td>2867</td>
<td>$\rightarrow$ CH$_3$CN + CH + H$_2$</td>
<td>3.3 x 10$^{-4}$</td>
<td></td>
</tr>
<tr>
<td>2868</td>
<td>HCCCO$^+$ + e $\rightarrow$ C$_2$H + O</td>
<td>1.9 x 10$^{-6}$</td>
<td></td>
</tr>
<tr>
<td>2869</td>
<td>CHOCHO$^+$ + e $\rightarrow$ HCO + CO + H</td>
<td>4.7 x 10$^{-8}$</td>
<td></td>
</tr>
</tbody>
</table>

Notes: (1) The rate coefficient is 6.84 x 10$^{-18}$√100/T.

2.5. Neutral-neutral reactions—excluded

Neutral-neutral reactions have typical reaction rate coefficients $k_N \sim 4 \times 10^{-11}$ cm$^3$s$^{-1}$ if they have no activation energy. Experimentally some reactions are known to have rate coefficients near $k_N$ under laboratory conditions ($T = \sim 300$ K). We have no means to predict whether a neutral-neutral reaction has an activation energy or not. Even if a reaction proceeds at the room temperature, it may have an activation energy $E_a \leq 300/k$ which affects the reaction rate under interstellar conditions. Our purpose in this paper is to clarify the ion chemistry in dense clouds. Thus, neutral-neutral reactions are neglected in this research.

One of the effects of neutral-neutral reactions is to convert radicals to molecules and create stable bonds. Especially, O-O bond is difficult to form in the ion-neutral reaction scheme because the OH$^+$ + O reaction has no exothermic channels such as O$_2$H$^+$ + H$_2$. The O + OH $\rightarrow$ O$_2$ + H reaction has a rate coefficient of $4 \times 10^{-11}$ cm$^3$s$^{-1}$ at 300K and may be the major source of O-O bond in dense clouds. As we exclude this reaction, we add OH$^+$ + O and H$_2$O$^+$ + O reactions though OH$^+$ and H$_2$O$^+$ are class II species. For the same reason, OH$^+$ + N and H$_2$O$^+$ + N reactions are considered for producing the N-O bond. In this case, it is less serious than in the case of O-O bond to neglect OH + N $\rightarrow$ NO + H reaction because NH$_3$ + O reaction produces N-O bond.

Finally, a chemical reaction model including 2885 reactions of 234 species (including e, He, He$^+$) have been constructed. The abundances of species are described by the following non-linear simultaneous differential equations,

$$
\frac{dx_i}{dt} = \sum_j a_{ij} x_j + \sum_k b_{ijk} x_j x_k n_H,
$$

(2.1)

where $a_{ij}$ are the rates of cosmic-ray bombardment reactions of $j$-th species (s$^{-1}$) and $b_{ijk}$ are the rate coefficients of collisional reactions between $j$-th and $k$-th...
species (cm$^3$s$^{-1}$). These equations are solved time-dependently by implicit-explicit time difference method. The conservation of the numbers of charge and each element is examined to see the accuracy of the calculations. For the case demonstrated in § 3, the errors $(\delta x_i/x_i)$ are $<10^{-2}$ and $<3 \times 10^{-6}$ for charge and element conservations, respectively, throughout the calculation. These small errors indicate that our method of calculations is reliable.

§ 3. Results and discussion

The molecular abundances obtained by the model calculation on the basis of the chemical reaction network in § 2 are demonstrated in Figs. 1(a) ~ (d). The cloud model is very simple: The number density and the temperature are fixed to be $10^5$ cm$^{-3}$ and 30K, respectively, all elements are in atomic form initially, the elemental abundances are cosmic, and the ionization rate of an H atom by cosmic rays, $\zeta_H$, is $10^{-18}$ s$^{-1}$.

The H$_2$ molecule has been produced to the amount $x$(H$_2$)~0.01 at $t$~$10^4$s and continues to increase $(d \log x$(H$_2$)/$d \log t$~1) until most H atoms are consumed $(t$~$10^{12}$s). As H$_2$ increases, overall rate of molecule formation becomes larger since reactions of ions with H$_2$ molecule are the main source of chemical bonds of the other molecules. Ions which first have been produced by cosmic-ray ionization are neutralized mainly by recombination of H$^+$ with electron until $t$~$10^8$s. Before H$^+$ and electron reach their steady states, the charge transfer of H$^+$ ion to molecules becomes faster than the recombination and Mg$^+$ ion becomes most abundant among ions. Electrons and ions attain their local steady states at $t$~$10^{11}$s and H atom, with H$_2$ molecule at $t$~$10^9$s. All species become in equilibrium at $t$~$2 \times 10^{18}$s, though this time far exceeds the lifetime of dense clouds ($10^{13}$ to $10^{16}$s).

Roughly speaking, heavier, more saturated neutrals begin increasing later than the lighter ones, but their growth curves are steeper than those of lighter ones. As a consequence, most of the neutrals in the chemical scheme are produced to the amounts $x_i$~$10^{-11}$ at $t$~$10^4$s, when the neutrals containing carbon (except those containing C-O bond) have a peak abundance. This is the time when C atoms are exhausted in forming CO molecules. As the C atom decreases, the neutrals containing carbon (except those containing C-O bond) decrease until the C atom attains its steady state at $t$~$10^9$s. These facts show that the existence of C atoms (consequently its hydrides and their ions) is essential to make the molecules longer and larger. The CO abundance in dark clouds and molecular clouds evaluated from $^{13}$CO observations shows that only $\leq 1/10$ of the solar abundance of carbon is in the form of CO, though this may be caused by the condensation onto grains and/or by the departure from the solar abundance. Variation of initial abundance ratio and/or inclusion of the depletion of elements will change the nature of molecular evolution in dense clouds. The effects of these factors
Fig. 1. Relative abundance $x_i = n_i/n_H$ ($n_H$ is the total nucleon number density which is taken to be $10^6 \text{ cm}^{-3}$) as a function of $\log t$, where $t$ is the time. Initially, all elements are locked up in atomic form. Because there are numerous species, they are divided into four figures, (a)~(d).
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will be discussed elsewhere.

We have neglected the condensation reactions of class II species. Parts of them are produced substantially. If we included condensation reactions of them, heavier neutrals \( \text{C}_m\text{H}_n \), \( \text{HC}_n\text{N} \), \( \text{C}_m\text{H}_n\text{CN} \), \( \text{C}_m\text{H}_n\text{OH} \), etc. should be synthesized to an extent comparable with observations.

To simplify the problem, we examine how reactions affect the molecular evolution. The total yield \( R = \int b_{ij} x_j n_i dt \) (or \( R = \int a_{ij} x_i dt \) for the case of cosmic-ray reactions) is calculated for each reaction. We set a critical ratio \( R_c \) and counted effective reactions which contribute to more than \( R_c \) of formation or destruction of at least one species. The most effective reaction for destruction or formation of a species is counted even if the contribution is less than \( R_c \). The dissociative recombinations are taken into account as an only producing process of neutrals. The numbers of effective reactions are 1596, 782 and 375 for \( R_c = 0.01, 0.1 \) and 0.3, respectively. We have calculated using 448 effective reactions for \( R_c = 0.2 \), which are tabulated in Table I, and found that the general feature and the abundances of major components do not change very much. The full lists are available on request.

The results cannot be compared directly with the observations because we have excluded neutral-neutral reactions and the contributions of grains. Some molecules are overabundant compared with the observations. Especially, the abundances of radicals (for example, HCO, CN and CH) far exceed the observational value. We expected that the radicals would be less abundant than the molecules because of the high heats of formation. The abundances of the radicals and the molecules which have the same configuration of heavy atoms are of the same order for most cases. We should conclude that ion-neutral reactions produce radicals as much as the molecules. The neutral-neutral reactions of more reactive radicals have smaller activation energies and will make the neutrals evolve to more stable neutrals. If neutral-neutral reactions were included in our scheme, the final abundances should change seriously. Especially, the C atom and the CH radical will be consumed by \( \text{C} + \text{OH} \rightarrow \text{CO} + \text{H} \) and \( \text{CH} + \text{O} \rightarrow \text{CO} + \text{H} \) reactions, respectively, to form CO. Grain surfaces will also have similar effects. Radicals may condense onto the grain surfaces more easily than molecules do because the adsorption energies should be greater for radicals than for molecules. Furthermore, surface reactions produce mainly molecules because energy supply from the reaction is sufficient to overcome the adsorption energy and to eject the products. These effects as well as the qualitative comparison with observations will be discussed in succeeding papers.

In spite of these uncertainties, we can conclude that ion-neutral reactions can certainly produce the observed molecules, though grain surfaces may also influence the molecular abundances. The most important part of molecular evolution should be attributed to the ion chemistry in the gas phase. The effects of variation of initial abundance, neutral-neutral reactions and grain surfaces will also be discussed later.
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References