# THE CHEMISTRY OF COOL CIRCUMSTELLAR ENVELOPES

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ABSTRACT. We have developed a time-dependent chemical kinetic model to describe the chemistry in the circumstellar envelopes of cool stars, with particular reference to IRC + 10216. Our detailed calculations show that ion-molecule reactions are important in the formation of many of the species observed in IRC + 10216.

## 1. INTRODUCTION

The envelope of IRC + 10216 is observed to contain many complex molecules nearly all of which have also been detected in the dark dust cloud, TMC-1. In this source, cosmic-ray ionisation drives the chemistry which, at least for the smaller molecules, is fairly well understood (Millar and Freeman 1984, Leung, Herbst and Huebner 1984). Ion-molecule chemistry can also occur in IRC + 10216 driven by both cosmic-rays and the external interstellar ultraviolet radiation field (Huggins and Glassgold 1982, Nejad, Millar and Freeman 1984). Parent species injected into the envelope at $r_0 = 10^{16}$ cm are CO, $C_2H_2$, HCN, $CH_4$, $NH_3$ and $N_2$, though this latter species has only a minor effect on the chemistry. These parents give rise to a system which totals 80 species whose radial abundances are calculated by integrating the resulting system of stiff differential chemical kinetic equations through use of the GEAR method. In Table 1 we present a summary of one of the many calculations performed by us.

## 2. DISCUSSION

The absorption of the external UV field by dust grains in the envelope ensures that at $r = 10^{16}$ cm the chemistry is driven by cosmic-ray ionisation of $H_2$. The $H_3^+$ ion so produced has a low proton affinity and undergoes proton transfer reactions with CO, $C_2H_2$, HCN and $NH_3$. The ion $HCO^+$ does not have a large abundance however because it transfers protons to $C_2H_2$, HCN and $NH_3$. The formation of $HCNH^+$ can lead to the production of HNC through dissociative recombination while



*I. Appenzeller and C. Jordan (eds.), Circumstellar Matter, 551–552.*

TABLE 1. Calculated column densities, N($cm^{-2}$), for IRC + 10216 using $\dot{M} = 5 \times 10^{-5}\ M_{\odot}\ yr^{-1}$ and $V_e = 16\ km\ s^{-1}$.

| Species | N | Species | N | Species | N |
|---|---|---|---|---|---|
| CN | 7.4(14) | $C_2H$ | 1.8(15) | $HCO^+$ | 1.7(12) |
| HCN | 2.1(13) | $C_3H$ | 5.5(13) | $HCNH^+$ | 1.8(12) |
| CCN | 4.4(11) | $C_3H_2$ | 5.7(13) | $CH_2CO$ | 6.0(11) |
| $C_3N$ | 5.2(12) | $C_4H$ | 2.1(14) | $CH_3CN$ | 1.0(13) |
| $HC_3N$ | 4.6(12) | $C_3O$ | 3.7(12) | $C_2H_3$ | 1.1(14) |

$C_2H_3^+$ reacts with $C_2H_2$, $CH_4$ and CO to form more complex species. As one proceeds outward in the envelope, the external UV dominates cosmic-rays and provides a source of ionisation as well as the creation of daughter species. In this region the chemistry is particularly interesting. The most important ions in driving the chemistry become $C_2H_2^+$, $CH_3^+$ and $C^+$. The ion $C_2H_2^+$ reacts with many species and leads to $C_3O$, $HC_3N$, $C_3N$, $C_4H$, $C_3H_2$, $C_3H$ and CCN. $CH_3^+$ reacts slowly with $H_2$ but has an extremely rapid radiative association with HCN and an association with CO which produce $CH_3CN$ and $CH_2CO$ respectively.

Our detailed calculations enable us to make the following conclusions about ion-molecule chemistry in IRC + 10216.

1. Cosmic-rays and UV radiation provide a source of ionisation which drives an extensive ion-molecule chemistry in the envelope.

2. Given the uncertainties in both the observationally derived column densities and those calculated theoretically, we find a good agreement between observation and theory for many species including CN, $C_2H$, HNC, $C_3H$, $C_3H_2$, $C_4H$ and $CH_3CN$.

3. The calculated abundances of $C_3N$ and $HC_3N$ are too low by more than an order of magnitude which may imply that they, or at least $HC_3N$, are formed in the warm, denser gas interior to $10^{16}$ cm.

4. Certain oxygen-bearing species such as $C_3O$, $CH_2CO$ and $HCO^+$ may be detectable in IRC + 10216.

5. Similarities between the chemical composition of TMC-1 and IRC + 10216 can be explained by the occurance of a similar ion-molecule chemistry in both objects.

6. Differences in the absolute abundances of certain species in these two objects relate to the fact that in IRC + 10216, the chemistry involves the breakdown of stable parent molecules into atoms and atomic ions, while in TMC-1 it involves the build-up of these parents from atoms.

## 3. REFERENCES

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