Microphysics and astrophysical observations: The molecular perspective

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Abstract. A general overview of the molecular content in interstellar clouds is reported. We concentrate on the role of dissociative recombination on interstellar chemistry. Recent observations are emphasized both in diffuse and dense clouds environments. Specific suggestions of theoretical and/or experimental studies on branching ratios involved in dissociative recombination experiments are highlighted.

1. Introduction
The recognition that molecules are an important component of the universe is recent. Sir A. Eddington [1] mentioned in 1937: I write about molecules with great diffidence, having not yet rid myself of the tradition that atoms are physics, but molecules are chemistry, but the new conclusion that hydrogen is abundant seems to make it likely that the above mentioned elements H, O, and N will frequently form molecules. However, molecules are now found in a variety of astrophysical environments, ranging from planetary atmospheres, comets, late type stars, circumstellar envelopes, protoplanetary disks and interstellar medium to extragalactic regions. The molecular gas in our Galaxy represents about 10% of its mass. Molecules are efficient coolers via their rotational radiative emission, thereby diminishing thermal support relative to self gravity and are thus the preferential sites of star formation. Neutral molecular gas also reduces the degree of ionization in molecular clouds and therefore decouples the gas from any supporting magnetic field.

Recent improvements of our knowledge on the molecular content have been obtained thanks to the availability of performant observational tools such as millimeter radiotelescopes and interferometers (IRAM, NRAO, Onsala), visible and infrared spectrographs on large telescopes (VLT) and UV facilities on spatial missions such as FUSE. There are presently more than 125 detected identified molecules, without counting isotopic substitutions involving deuterium, $^{13}$C, $^{18}$O, $^{17}$O, $^{15}$N, $^{29}$Si, $^{34}$S, $^{33}$S, etc. Table 1 displays the present list of species identified in interstellar and circumstellar regions, most of which were detected via millimeter, sub-millimeter and infra-red emission. Italic symbols refer to detections via electronic transitions in the UV or visible wavelength range which are possible in the diffuse or so-called translucent clouds. Molecular ions, very important tracers of the ionization state of the environment, appear in bold face. Molecules detected only in circumstellar environments are labelled with an asterisk whereas molecules detected both in the interstellar medium and circumstellar environments are labelled with 2 asterisks. In addition, molecules detected in external galaxies are underlined. The consideration of table 1 clearly shows that a specific chemistry is at work as many reactive species, molecular radicals, carbon chains, unstable isomers are readily found in addition to saturated, well known terrestrial molecules.
Table 1. Interstellar and circumstellar molecules

| Species with only Hydrogen atoms |  |
|---------------------------------|--|
| $\text{H}_2$∗∗                | $\text{H}_3^+$               |

Molecules containing Carbon and Hydrogen

| CH                | C$_2$H$_2^+$ | C$_3$H$^+$ | CH$_4$** | c-C$_3$H$_2$** | l-C$_3$H$_2^+$ | c-C$_3$H$^+$ |
|------------------|-------------|-----------|----------|----------------|----------------|------------|
| C$_2$H$_3$** | C$_2$H$_2$** | CH$_3$CCH$^+$ | C$_2$H$_4$ | l-H$_3$C$_4^+$ | C$_4$H$^+$ | CH$_5^+$ |
| CH$_3$CCH$^+$**| C$_6$H$^+$ | C$_6$H$_2$** | HC$_6$H$^+$ | C$_7$H$^+$ |
| CH$_3$C$_4$H$^+$ | C$_8$H$^+$ | C$_6$H$_6$^+ |

Molecules containing Carbon and Hydrogen

| CH$_4$** | C$_2$H$_2$** | C$_3$H$^+$ | CH$_3$CCH$^+$ | C$_6$H$^+$ | C$_6$H$_2$** | HC$_6$H$^+$ | C$_7$H$^+$ |
|----------|--------------|------------|---------------|------------|--------------|------------|------------|
| C$_2$H$_3$ | C$_2$H$_2$** | CH$_3$CCH$^+$ | C$_2$H$_4$ | l-H$_3$C$_4^+$ | C$_4$H$^+$ | CH$_5^+$ |
| CH$_3$CCH$^+$** | C$_6$H$^+$ | C$_6$H$_2$** | HC$_6$H$^+$ | C$_7$H$^+$ |
| CH$_3$C$_4$H$^+$ | C$_8$H$^+$ | C$_6$H$_6$^+ |

Molecules with Oxygen and/or Hydrogen and Carbon

| CH$_2$O** | HCO$^+$ | CO$^+$ | C$_2$O | H$_2$O** | HCO | H$_2$O$^+$ |
|-----------|---------|-------|------|----------|-----|-----------|
| HCO$^+$ | HOC$^+$ | C$_2$O | C$_3$O | HCOOH | CH$_2$CO |
| HCO$^+$ | H$_2$CO$^+$ | C$_3$O | C$_3$O | HCOOH | CH$_2$CO |
| H$_2$COH$^+$ | CH$_3$OH$^*$ | CH$_3$CHO | HC$_3$CHO | C$_5$O |
| CH$_3$CHO | C$_2$H$_2$O | CH$_3$CHO | CH$_2$OHCHO | CH$_3$COOH |
| CH$_3$CHOH | (CH$_3$)$_2$O | CH$_3$CHCHO | CH$_3$CH$_2$CHO | CH$_3$CH$_2$CHO |
| CH$_3$CH$_2$OH | (CH$_3$)$_2$CO | HOCH$_2$CH$_2$OH | C$_2$H$_5$OCH$_3$ |

Molecules with Nitrogen and/or Hydrogen and Carbon

| NH | CN$^*$ | N$_2$ | HC$_3$N$^+$ | HCN$^*$ | HNC$^*$ |
|----|-------|------|------------|--------|--------|
| N$_2$H$^+$ | NH$_2^+$ | HCN$^+$ | HCN$^*$ | HNC$^*$ |
| C$_3$N$^*$ | CH$_2$CN | CH$_2$NH | HC$_3$N$^+$ | HCN$^*$ |
| NH$_2$CN | C$_3$NH | CH$_3$CN$^*$ | CH$_3$NC | HCN$^*$ |
| CH$_3$CN | CH$_3$CN | CH$_2$CN | HC$_3$N$^+$ | HCN$^*$ |
| C$_2$H$_5$CN | HC$_3$N$^*$ | CH$_3$CN | HC$_3$N$^+$ | HCN$^*$ |
| C$_2$H$_5$CN | HC$_3$CN | CH$_3$CN | HC$_3$N$^+$ | HCN$^*$ |

Molecules with Nitrogen and Oxygen

| NO | HNO | N$_2$O | HNCO | NH$_3$CHO |
|----|-----|------|------|---------|

Molecules containing Sulfur, Silicon or one metallic atom

| SH | CS$^*$ | SO$^*$ | SO$^+$ | NS | SiH | SiC | SiN$^*$ | SiO$^*$ | SiS$^*$ |
|----|-------|-------|-------|----|----|----|--------|--------|--------|
| HCl | NaCl$^+$ | AlCl$^+$ | KCl$^+$ | HF | AlF$^+$ | PF$^*$ | PN$^*$ | H$_2$S$^*$ | C$_2$S$^*$ |
| SO$_2$ | OCS | HCS$^+$ | c-SiC$_2$ | SiCN$^*$ | NaCN$^+$ | MgCN$^*$ | MgNC$^*$ | H$_2$CS | HNCS |
| C$_3$S$^*$ | c-SiC$_3$ | SiH$_4^*$ | SiC$_4^*$ | CH$_3$SH | C$_5$S | FeO | AlNC$^*$ |
interactions. The present review will focus on pure gas phase chemistry.

2. Modelling strategy

2.1. Astrophysical parameters

Modelling of any interstellar cloud implies a drastic simplification of the environment. The main astrophysical parameters introduced in a chemical model are summarized below:

- Choice of a specific geometry
- Density profile, elemental abundances
- Energy input: cosmic ionization rate, interstellar UV radiation field, mechanical energy
- Dust properties: albedo, opacity, size distribution, composition, volumic mass, dust to gas mass ratio
- Chemical network with appropriate reactions
- Heating and cooling mechanisms

Chemical balance may be expressed for each atomic and/or molecular species labelled $i$ as

$$\frac{dn_i}{dt} = F - Dn_i$$

where $F$ stands for all formation processes involving reactions between the other species, and $D$ represents the destruction processes. The resulting coupled differential equations may be solved for specific initial conditions so that one follows the chemical evolution until steady state. It is also possible to solve directly $\frac{d}{dt} = 0$ to obtain the steady state solution(s).

2.2. Basic molecular processes

The description of the chemical mechanisms taking place in interstellar conditions is given in several reviews (e.g. [2]). Both gas phase and surface reactions may be at work. Gas phase processes pertaining to interstellar conditions involve essentially binary and exothermic chemical reactions. The ion-molecule scheme introduced by Herbst and Klemperer [3] has been extremely successful with the detection of polyatomic molecular ions in interstellar clouds. Dissociative recombination is of major importance as it establishes the nature and amount of neutrals finally released in interstellar environments. There is however no doubt that surface reactions on interstellar dust grains also take place although the corresponding quantitative studies are much more difficult than for gas phase processes. The presence of $\text{H}_2$ can indeed not been accounted for without reactions on grain surfaces.

3. Importance of dissociative recombination in diffuse and translucent cloud chemistry

Two recent observational results may be emphasized in relation with dissociative recombination.

- The $\text{H}_3^+$ molecular ion puzzle

Detection of $\text{H}_3^+$ towards a standard diffuse cloud such as $\zeta$ Per [4] has raised one more time the importance of the dissociative recombination of the $\text{H}_3^+$ molecular ion. The authors report another experimental determination of the corresponding rate coefficient via the CRYRING storage ring, where careful analysis of the initial rotational state of the molecular ion is performed, leading to a value of the rate coefficient of $2.6 \times 10^{-7}$ cm$^3$ s$^{-1}$ at astrophysically relevant temperatures, in agreement with the most recent theoretical calculations [5]. From this measurement, McCall et al. [4] infer a cosmic ionization rate 25 times higher than the currently assumed value of about $5 \times 10^{-17}$ s$^{-1}$, which has significant consequences on the chemical environment of $\zeta$ Per and raises the question of the origin of this enhancement. Le Petit, Roueff and Herbst [6] have analyzed all the observational and physical constraints, including the new determination of the $\text{H}_3^+$ dissociative recombination, and conclude that a simple homogeneous cloud is incompatible with
the observations. The main conclusion is that a dense clump has to be present on the line of sight in order to account for the presence of C$_2$ and C$_3$ which have been detected in this line of sight. Alternatively, a cosmic ray ionization of $2.5 \times 10^{-16}$ s$^{-1}$ is inferred, which allows to reproduce at a reasonable level the observed column densities of OH and HD, both species being very sensitive to the value of the cosmic ionization rate.

- Detection of N$_2$ towards HD124314

Knauth et al. [7] report the detection of N$_2$ towards the HD124314 translucent cloud in an ultra-violet spectrum obtained via FUSE, in addition to H$_2$, HD, CO, neutral atomic sulfur and nitrogen. Interpreting this detection is very challenging as a recent measurement of the dissociative recombination of N$_2$H$^+$ by Geppert et al. [8] reports that N$_2$ is not the main product as usually believed. Preliminary calculations using the “PDR” code dedicated to translucent regions and photon-dominated regions by Le Petit, Roueff and Le Bourlot [9] have been performed in order to test the formation of molecular nitrogen in such appropriate physical conditions, by using the recent molecular data. However, it was found again that a single homogeneous model is not able to reproduce the observed amount of molecular nitrogen.

These two examples emphasize the importance of reliable molecular data for astrophysicists, as essential prerequisites for a real physical discussion of the considered environments.

4. Is it possible to infer branching ratios?

Most polyatomic species, found in cold and dense clouds, are neutral. In the ion-molecule gas phase chemistry, neutral molecules are the products of dissociative recombination of polyatomic molecular ions so that the knowledge of the various branching ratios is decisive. Various ion storage ring experimental studies have been able to measure the branching ratios of different molecular ions. The 3-body dissociation channel into H + H + X of a XH$_2^+$ molecular ion (with $n \geq 0$) is found to be significant. Figure 1 displays the branching ratios of different molecular ions as a function of the exothermicity of the reaction. A former example of this curve had been displayed in [10] at the previous meeting and the present curve has been revised according to the recent measurements. The branching ratio toward a three body break up increases with the exothermicity of the reaction and follows a power law as displayed in figure 1.

The generalization to other molecular ions is appealing but conjectural. Future experimental and/or theoretical studies are required.

![Figure 1. Branching ratio towards 3-body ejection of polyatomic ions as a function of the exothermicity expressed in eV.](image-url)
Table 2. Deuterated molecules detected in the interstellar medium.

| Molecule       | Deuterated Species |
|----------------|--------------------|
| HD*            | HDCO               |
| HDO†           | HDCS               |
| DCO+           | ND2H               |
| DCN†           | DC3N               |
| D2CO           | CHD2OH             |
| DCS            | CH3OD              |
| HDS            | CH2DOH             |
| C2D            | ND3                |
| C4D            | CH2DCC             |
| C3HD           | CD2OH              |
| NH2D           | CH3D°              |

* HD has been detected in planetary atmospheres, comets and in the interstellar medium thanks to its rotational transition at 112 µm and through UV absorption in diffuse and translucent interstellar clouds as well as in front of a distant quasar where the UV Lyman transitions of HD are shifted in the visible range.
† also detected in comets
○ only detected in planetary atmospheres

5. Deuterated gas phase molecules

5.1. Observational status

Detection of deuterated species has been a very active field of research these past years (e.g. [11]) and table 2 displays the species presently detected in cold astrophysical environments. Molecular ions deserve special attention and are displayed in the third column. The most unexpected and surprising recent detections are that of the multiply deuterated species which have been found in low mass star forming regions and dark interstellar clouds. Whereas the cosmic D over H ratio is about $1.5 \times 10^{-5}$, the deuterated isotopolog over normal species column densities ratio is considerably enhanced:

$$XH/XD \simeq 10^{-1} - 10^{-3}$$
$$XD_2/XH_2 \simeq 10^{-2} - 10^{-3}$$
$$XD_3/XH_3 \simeq 10^{-3} - 10^{-5}$$

5.2. H2D+ and D3H+

Deuterium enhancement of monodeuterated species has been recognized since more than 30 years [12] as a result of chemical fractionation due to the difference in zero point energies of the deuterated and hydrogenated molecules. The key reaction is the deuteron exchange in the reaction between HD, the reservoir of deuterium in dark interstellar clouds, and the H3+ molecular ion: $H_3^+ + HD \leftrightarrow H_2D^+ + H_2$. The low temperature conditions present in the interstellar medium favor the left-to-right reaction as the energy difference involved is 232 k, where k is the Boltzmann constant.

This reaction competes with dissociative recombination and other ion-molecule reactions involving abundant species, such as O, CO etc. The importance of the dissociative recombination of the H3+ molecular ion is emphasized once more. However, the occurrence of multiply deuterated species have incited different authors to proceed further and consider the subsequent reaction of H2D+ with HD, leading to D2H+ (detected in a prestellar cloud by Vastel et al. [13]), which can further react with HD, giving D3+. Figures 2 and 3 display the various energy levels (not at scale) which may be involved in the reaction as well as their related ortho/para characters. Also shown are the H2D+ and D2H+ emission transitions detected in the cold dense pre-stellar core L1544 by Caselli et al. [15] and Vastel et al. [13], respectively. It is remarkable that these both transitions arise from levels above 80 K whereas the temperature of the cloud is around 10 K. The occurrence of a “state to state” chemistry could be at work. The fundamental transitions connecting the ground rotational levels are in the Terahertz domain and are observational candidates for the HIFI instrument [14] on Herschel as shown in the figure. In so called depleted regions where CO, O and H2O are trapped on grains, the reactions cited above are very efficient in building multideuterated hydrogen ions and are balanced only by dissociative recombination. Such completely depleted core conditions have been considered by Walmsley, Flower and Pineau des Forêts [16].
5.3. Dissociative recombination of partially and totally deuterated molecular ions

Some experimental studies on dissociative recombination have been performed on partially deuterated molecular ions [17–19] and the corresponding branching ratios are displayed in figure 4. Obviously the ejection of atomic hydrogen is about twice more efficient than the ejection of D, which favors the building of deuterated species. This result is different from the current hypothesis of equipartition used in most astrophysical models. Marcelino et al. [20] have assumed that a ratio of 2 : 1 for the ejection of H compared to D is occurring in the dissociative recombination of all molecular ions included in the chemical network in order to interpret, via a gas phase model, the detection of deuterated isotopologs of thioformaldehyde (HDCS and D₂CS). It is important to mention that a significant depletion factor for C and O is also required to obtain satisfactory agreement between models and observations.

Experimental information on such branching ratios is thus very welcome. Most interesting candidates for astrophysical applications are H₂DO⁺ and all deuterated isotopologs of NH₄⁺, H₃S⁺, H₂CS⁺ etc. The knowledge of the absolute values of the total rates is also an important issue. Table 3 displays the total
reaction rate coefficients for three completely hydrogenated and deuterated molecular ions. The reaction rate coefficients decrease when deuterium replaces hydrogen. This fact also favors the formation of multideuterated species in the gas phase. Is this trend general?

5.4. DCN/HCN and DNC/HNC

The DCN/HCN and DNC/HNC abundance ratios deserve some special comments. In dark cloud conditions, the general trend that DCN/HCN is smaller than DNC/HNC is noticeable [11]. The common hypothesis that interstellar HCN and HNC are produced with equal amount from the dissociative recombination of HCNH$^+$ is plausible and supported by theoretical ab-initio calculations [24]. The isomer ion H$_2$NC$^+$ leads to HNC only. However, when deuterated substitutes are introduced, more caution is recommendable. The reaction channels displayed in table 4 are based on the assumption that no rearrangement of the atoms occurs during the recombination process.

As potential energy surfaces of the HCNH$^+$ ion have been obtained by Taketsugu et al. [24], it is then highly desirable that theoretical dynamical calculations may tackle this problem. In addition, the production of DCN and DNC may be enhanced if the ejection of H is privileged in the dissociative recombination, as discussed above.

Figure 5 shows the results of a model used by Roueff et al. (to be submitted) when the 2 : 1 hypothesis is made for the branching ratio of deuterated species, as described above. Each point in figure 5 refers to a steady state result obtained at a specific temperature for a cloud model appropriate to dense core conditions: $n$(H$_2$) = $10^3$ cm$^{-3}$, with a cosmic ray ionization rate $\zeta$ of $2 \times 10^{-17}$ s$^{-1}$. On the other hand, a substantial depletion is assumed compared to the “standard” TMC1 cloud, i.e. C/H$_2$ = $1.4 \times 10^{-5}$, N/H$_2$ = $2 \times 10^{-5}$ and C/O = 0.35. Only gas phase processes are considered (except for H$_2$) and grains are assumed to be passive as the elemental abundances chosen imply that a significant amount

| Molecular ion | dissociative recombination reaction rate coefficient [cm$^3$ s$^{-1}$] | Reference |
|--------------|-------------------------------------------------|-----------|
| H$_3^+$      | $6.8 \times 10^{-8}$ (T/300)$^{-0.5}$           | [4]       |
| D$_3^+$      | $2.7 \times 10^{-8}$ at 300 K                   | [21]      |
| H$_3$O$^+$   | $7.6 \times 10^{-7}$ (T/300)$^{-1.1}$           | [22]      |
| D$_3$O$^+$   | $7.6 \times 10^{-7}$ (T/300)$^{-1.1}$           | [22]      |
| NH$_4^+$     | $9.43 \times 10^{-7}$ (T/300)$^{-1.25}$         | [23]      |
| ND$_4^+$     | $5.67 \times 10^{-7}$ (T/300)$^{-0.687}$        | [23]      |

Table 4. Assumed reaction channels in the dissociative recombination reactions of deuterated HCNH$^+$ and H$_2$NC$^+$

| Reaction Channel | Products |
|-----------------|----------|
| HCND$^+$ + e$^-$ → HCN + D | DNC + H |
| DCNH$^+$ + e$^-$ → DCN + H | HNC + D |
| HDNC$^+$ + e$^-$ → HNC + D | DNC + H |
of CO, O and H₂O is trapped on grains. The chemical network used includes 210 species including up to 5 deuterium atoms but limited to three C containing molecules as the main goal of the study is focussed on ammonia and thioformaldehyde. 2960 reactions have been used which include the recent updated values of dissociative recombination rate coefficients. The DCN/HCN values are smaller than the DNC/HNC for temperatures below about 20 K and decrease with temperature as fractionation reactions become less efficient at higher temperatures. This result is in agreement with the observations in cold regions reported by Roueff and Gerin [11]. As the deuterium enhancement decreases at higher temperatures, the prediction that DNC/HNC becomes smaller than DCN/HCN above 20 K is difficult to test observationally. Such attempts would however be interesting in order to probe the chemical model.

6. Conclusions

Some examples of the interplay between detailed molecular processes and astrophysical observations have been discussed with special emphasis put on dissociative recombination reactions. Collaboration between the communities is very fruitful as observations drive new and unexpected problems. Sensitivity analysis of the model results on the molecular data should be kept in mind as discussed in previous meetings [10]. The status of the chemical complexity present in interstellar clouds will remain an important problem in the forthcoming years.

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