Molecular carriers in the ISM

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ABSTRACT

We will carry out a comprehensive spectroscopic study of molecular carriers, probing interstellar hydrides and carbon chain and ring molecules. Our investigation of hydrides will entail high-resolution HIFI spectroscopy of some 20 hydride and deuteride molecules towards 18 bright continuum sources, together with complementary observations with PACS and SPIRE. The list of target hydrides includes molecules containing the elements C, N, O, F, Cl, and Fe. We will detect multiple absorption components from foreground gas clouds of diverse properties that are known to intersect the selected lines-of-sight, along with emission and absorption intrinsic to the background continuum sources themselves. Our investigation will provide a wealth of new information about the abundances of the interstellar hydrides – addressing key puzzles posed by previous observations from the ground and with ISO, SWAS, and ODIN – and leaving an important Herschel legacy to astrochemistry and interstellar medium science. In particular, we will address the role of high temperature chemical reactions in the formation of interstellar molecules, and the question of how such reactions might be driven by heating mechanisms such as shock waves and interstellar turbulence. Our study will also elucidate the role of grain surface reactions in interstellar chemistry, reactions that are likely critical in controlling the inventories of molecular materials available within nascent planetary systems. We will investigate the growth of carbon molecules, bridging the gap between molecules and aggregates. FIR spectroscopy has the unique capability of enabling the detection of bending modes of large carbon molecules (chains or rings, possibly PAHs), securing their spectroscopic identification. Many of the absorption lines that are detectable only with Herschel in the local Universe become accessible to ground-based observatories at moderate to high redshift. Thus, absorption lines in quasar spectra are a potential probe of molecular gas at high-z; in the submillimeter spectral region, the high sensitivity of ALMA will generally be required. Herschel observations of absorption in the local Universe will provide an important benchmark for the future observations at high redshift that will become possible with ALMA.

Table 1: Diffuse ISM species

Detected species							
H_2	HD	H_3^+	CH	CH^+	CH_3	OH	H_2O
NH	NH_2	NH_3	H_2S	HF	HCl		
C_2	C_3	CCH	c-C_3H_2	CN	HCN	HNC	
CO	CO^+	HCO^+	HOC^+	H_2CO	CH_3OH	CH_3	
HCS^+	CS	SO	SiO				

Unknown carriers of detected spectral features	
DIB carriers	AIB carriers (PAHs)

1 Introduction

Among the many molecules identified in the interstellar medium and circumstellar envelopes so far (over 120, including isotopologues bearing rare isotopes such as Deuterium, ^{13}C, ^{18}O and ^{17}O, etc.) a significant subsample has been detected in the diffuse interstellar medium, ranging from H_2 and HD (Rachford et al. 2002) to rather complex species such as C_3 (Oka et al. 2003), and c-C_3H_2 (Lucas and Liszt 2000).

Molecules are found in the so-called "Cold Neutral Medium", where the kinetic temperature ranges from a few tens to one hundred Kelvins, the gas density ranges between a few hundred and a few thousands cm^{-3}, and the velocity dispersion is about 1 kms^{-1}. The average pressure $\sim 3 \times 10^3$ Kcm^{-3}, with large excursions above the median, up to 10^5 Kcm^{-3} (Jenkins & Tripp 2001). The sensitivity of the visible and FUV observations is such that the extinction threshold for detecting H_2 has been extended from $A_V \sim 0.1mag$ up to $A_V \sim 3mag$ (Rachford et al. 2002). Electronic transitions of a few other molecules are detected with very high sensitivity in the UV/visible/infrared, the most common being CO, CH, CH^+, CN, C_2, C_3 and H_3^+. Liszt and Lucas (2001 and references therein) have used background radio sources for detecting many additional molecules in the diffuse ISM, including OH, HCO^+, HCN, H_2CO, CCH, and c-C_3H_2.

The standard framework of the diffuse interstellar medium chemistry is fairly simple because of the rather low gas density, which limits the efficiency of chemical reactions for building molecules, and because the interstellar

FUV radiation efficiently destroys molecules. In this framework, molecules are built from atoms and ions in a series of two body chemical reactions, and the set of reactions can be solved assuming steady state. The whole set of chemical reactions is called a chemical network. At the moderate temperatures encountered in the diffuse ISM, exothermic reactions without activation barriers are preferred for building the chemical network. Endothermic reactions, reactions with activation barriers, and radiative associative reactions, which have much smaller rates, are included in a few cases, when these reactions are the sole routes for forming the interstellar species. It is therefore expected from the chemical models, that a restricted set of small and light molecules can be formed in the diffuse ISM, and that the chemistry is not efficient in building complex molecules (i.e. molecules with three or more heavy atoms).

However, even for low extinction lines of sight, simple chemical models encounter serious difficulties for reproducing observed molecular abundances. The failure occurs not only for the reactive ion CH^+ – which has a very specific chemistry, see below – but also for OH and HCO^+ whose chemistry is thought to be well understood, at least in dense, shielded gas (Liszt and Lucas 1996). The unexpected detection of the simple species H_3^+ (McCall et al. 2003) also does not fit in the standard framework. The diffuse interstellar medium therefore appears to be more chemically active than expectated based on steady-state chemical models. To proceed, the chemistry has to tap the large reservoir of non-thermal energy provided, for instance, by supersonic turbulence. Transient velocity and density structures, driving the dissipation of turbulence, certainly impact the chemistry, either by locally heating the gas well above its average value, or by generating large ion-neutral drifts. (e.g. Flower & Pineau des Forêts 1998; Joulain et al. 1998). Velocity resolved line profiles are a prerequisite for understanding the chemistry, as they provide simultaneous constraints on the molecular abundances, physical conditions and velocity field.

In addition, many spectral features remain unidentified in all wavelength ranges. For instance, the carriers of the strong spectral features seen in absorption in the visible spectrum of mildly reddened stars, and known as the Diffuse Interstellar Bands (DIBs) remain unknown despite many decades of active research. Large molecules made of carbon are the best candidates to account for the DIBs. They can be found in different forms such as carbon chains, rings, fullerenes or polycylic aromatic hydrocarbons (PAHs). The former are best detected in the far infrared via their ro-vibrational transitions (eg Cernicharo et al. 2002), the latter are good candidates to account for the so-called "unidentified"or aromatic infrared bands, observed in emission between 3 and 17 μm in many places of our Galaxy, as well as in external galaxies. Large carbon molecules play important roles both in the physics and chemistry of interstellar gas. One of the main gas heating process is the ejection of energetic electrons from dust grains via the photo-electric effect. The smallest particles are most efficient at releasing electrons. The contribution of large molecules, as PAHs, is essential for heating the interstellar gas to observed temperatures (e.g. Wolfire et al. 2003). As important reservoirs of carbon and charge carriers, PAHs impact the gas chemistry, but quantitative estimates are difficult without spectroscopic identifications, as the chemical processes can be very specific to individual PAHs .

The understanding of the ISM clouds must include the full range of sizes of ISM line carriers, from the smallest molecules (H_2 and hydrides) to the carbon clusters and PAHs. The opening of the full far-infrared and submillimeter wavelength domains by Herschel will provide a unique opportunity for progress in astrochemistry, because it gives access to important classes of key interstellar species, which have not been studied with heterodyne techniques before. The list includes the rovibrational transitions of large carbon molecules and carbon clusters, either with chains, rings or aromatic structures, which are very specific of the identity of their carrier, together with the ground state transitions of most hydrides. The line strength of the ground state transitions of these light polar molecules is such that they can be probed in the far infrared and submillimeter wavelength range with a high sensitivity, matching the sensitivity of optical observations : a typical figure is a line centre opacity of unity for a column density of 10^{13} cm^{-2} and a line width of 1 kms^{-1}.