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The Astrochemistry of Diffuse Interstellar Clouds

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Abstract. This paper provides an overview of the current research activity at the AstroChemistry Group (ACG) of the Astronomical Observatory of Cagliari (OAC) in the National Institute for Astrophysics (INAF).
Our team has been growing up since late '80s: from our first observations of Diffuse Interstellar Bands (DIBs), several related topics became part of the ACG scientific interests. DIBs' studies spurred many ideas which were developed during graduate and PhD studies, as the initial observational expertise was expanded to include numerical modelling and laboratory experiments.
We here present some highlights of our most recent results.

Key words. Astrochemistry — ISM: lines and bands — ISM: molecules — Molecular processes — Molecular data — Radiation mechanisms: general — Radiative transfer — Scattering — Methods: numerical

1. Introduction

The Diffuse Interstellar Medium (DISM) exhibits complex and intriguing facets, two of which constitute a *fil rouge* of the ACG activities: a set of spectroscopic features which lack a carriers' identification and the clumpy denser structure inside DISM. Regarding the latter, evidence for subparsec– scale structure in the DISM rapidly accumulated over the past few years, and remarkable observations exist showing complex molecules to achieve dark–cloud abundances in the DISM, possibly suggesting the presence of transiently very dense and hot regions at low overall extinction. The incorporation of density fluctuations, length-scale and filling factor in theoretical models of the DISM could be crucial to our understanding of DISM chemistry.

Diffuse Interstellar Bands and Unidentified Infrared Bands are two classes of spectroscopic features which claim, after so long time, a reliable answer about their origin. In this case, a robust computational activity is needed, shortly described during this paper.

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2. Chemical models

Despite the long history of gas– phase chemical modelling (see Watson, 1976; van

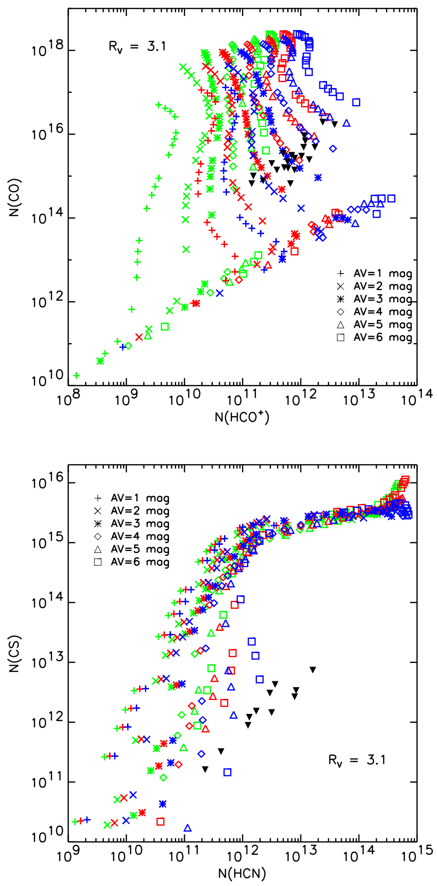

Fig. 1. *Top panel*: correlation between HCO^+ and CO column densities for different values of gas density and visual extinction for R_V = 3.1; *Bottom panel*: the same for N(HCN) and N(CS). The meaning of each symbol is reported in the legend. Black filled triangles show observational data as reported by Lucas & Liszt (2000); Liszt & Lucas (2001, 2002). Green: T = 25 K; red: T = 50 K; blue: T = 100 K

Dishoeck & Black, 1986; Zsargó & Federman, 2003, and references therein) and the large amount of observational work, some long–standing enigmas and a few recent failures push for a re– visitation of commonly accepted schemes and hint that diffuse clouds are much more complex than usually assumed. Among these enigmas, observations show that complex molecules may achieve dark– cloud abundances in the DISM. The interpretation of such a phenomenon is still lacking a robust observational scenario and it is doubtful whether present theoretical models may be reconciled with observed column densities. To assess this uncertainty, we are exploring the applicability of the standard gas-phase chemistry to the physical interpretation of observations in diffuse and translucent clouds. We computed an extensive grid (~4500) of depth–dependent, quiescent, steady– state chemical models, exploring the dependences of the predicted column densities on a wide range of several physical parameters (T_{kin}, A_V, R_V, $n_H = n(H)+2n(H_2)$), representative of the common definition of "diffuse molecular" medium. Our adopted chemical network has been constructed from 170 species consisting of the elements H, He, O, C, S and N. We selected from the UMIST data file (Millar et al., 1997) all the relevant reactions, updating some dissociative recombination rates with values from more recent literature. We assumed a plane parallel geometry for all the modelled clouds. The model cloud is illuminated by a normally incident UV radiation field, whose intensity is given in Draine (1978). The cosmic-ray ionization rate was assumed to be $\zeta=3\times10^{-17}$ s^{-1}.

We computed the column density of each species included in the network for all the possible combinations of physical parameters. As an example, Fig.1 shows the expected correlation between N(CO) and N(HCO^+)(upper panel) and between N(HCN) and N(CS) (lower panel) for a subset of physical parameters (see caption): the results are compared with the observed correlation (Liszt & Lucas, 2002).

The comparison between model results and observations suggests that standard chemical routes produce too low values of the HCO^+ column density and fail miserably to reproduce the observed column density of CS.

Similar considerations can be made for other molecular species, the main result being that standard chemical models in the physical conditions usually considered as typical of diffuse clouds (T = 100 K, $n_H \le 100$ cm^{-3}, $A_V < 2$ mag) are unable to meet the observa-

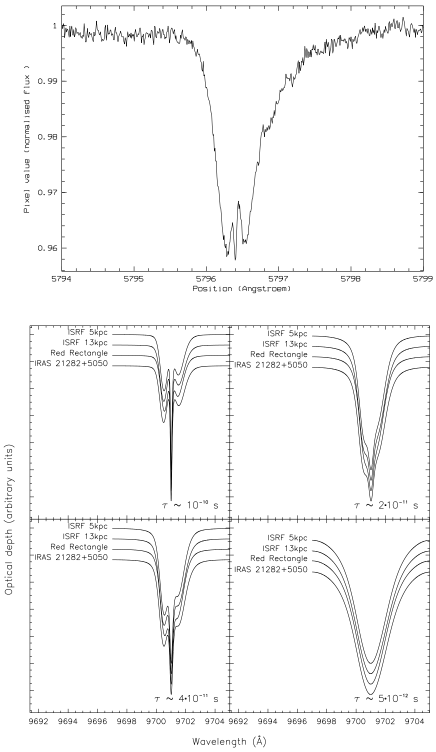

Fig. 2. *Top panel*; *Bottom panel*:

tional constraints. More specifically, there is no possible combinations of plausible physical parameters which may explain the observed column densities *in a global scenario*.
The final goal of this line of research is the creation of a large database of chemical results (photodissociation rates, volume and column densities, etc..) for a very large range of physical conditions. The final database will be available online in our web page (www.ca.astro.it and www.ars-network.org).

3. Molecular complexity of the ISM

A substantial fraction (about 80%) of the ~130 molecules identified in interstellar/circumstellar regions and solar system bodies, as well as a significative component of interstellar dust grains are carbon– based (see e. g. Ehrenfreund & Charnley, 2000). The realization that some unidentified, ubiquitous molecular spectral features are probably related to carbon in space gave rise, in the past few years, to intensive investigation on this subject. Among these *Unidentified Interstellar Features* are:

- The Aromatic Infrared Bands (AIBs), emission bands seen in the infrared near 3.3, 6.2, 7.7, 8.6 and 11.3 μm, observed along a large number of interstellar sight–lines covering a wide range of excitation conditions in numerous galactic objects as well as in external galaxies (Allamandola etal., 1989).
- The Diffuse Interstellar Bands (DIBs), a set of about 300 absorption features superimposed on the interstellar extinction curve and falling in the near– UV, visible and near– IR spectral range, with wavelengths from ~ 4000Å to ~ 10000Å (Herbig, 1995).

Both DIBs and AIBs are generally ascribed to large free– flying molecules in the diffuse ISM. In particular, AIBs have been hypothesized to originate in transitions involving the vibrations of CH and CC bonds in Policyclic Aromatic Hydrocarbons (PAHs). Molecules of this family, or other large carbon– bearing species, were subsequently proposed as carriers of at least some of the DIBs: in the so– called "strong" PAH hypothesis, these molecules are supposed to absorb Vis/UV radiation (hence producing DIBs), undergo internal energy conversion among the vibrational levels and subsequently relax by IR emission in their IR–active modes of vibration (hence producing AIBs). Despite intensive research, no specific interstellar PAH has been identified yet.

A detailed model of the interstellar photophysics of these elusive molecules may help to interpret observations and hopefully permit their eventual identification (Mulas, 1998; Malloci et al., 2003; Mulas et al., 2003, 2004). We have undertaken a long– term project, which spans from theoretical to laboratory to observational work aimed at:

- comparing optical synthetic spectra with available high– resolution DIBs observations obtained in the past decade, as well as with new *ad hoc* ones.

– comparing the IR synthetic spectra with the wealth of spectroscopic data collected in the past years by ISO, in particular in the far– IR spectral range. This comparison will already provide indications for the strategic planning of future Herschel observations.

This line of research is based on the use of a computational Monte Carlo model (Mulas, 1998) which simulates the photophysics of an isolated PAH molecule in the ISM. This computer code uses available experimental or quantum– chemical results to derive the rotational profiles of absorption bands (directly comparable to astronomical observations of DIBs) and the detailed IR emission spectra following the UV/Vis excitation. This yields many independent, simultaneous constraints on DIB spectral profiles, positions and equivalent widths, as well as on the absolute IR emission fluxes. While none of these pieces of information is sufficient *per se* for a specific molecular identification, when considered together they provide an unprecedented, unambiguous fingerprint.

We are now in the process of creating an atlas of modelled PAHs using an end– to– end computational machine which integrates *ab initio* available quantum chemistry codes and our Monte Carlo model.

4. Conclusions

Evaluation of the complex processes which arise into the DISM require an interdisciplinary activity, linking theoretical models, observational data and numerical simulations. Starting from DIBs' hunting, the AstroChemistry Group in Cagliari is evolving in this direction, as shown by the two sample projects outlined above.

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