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NEWSLETTER ON ANALYSIS OF ASTRONOMICAL SPECTRA

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Contents

Proceedings of the 1st Franco-British Meeting on
the Physics and Chemistry of the Interstellar Medium
Université des Sciences et Technologies de Lille, Villeneuve d'Ascq, France
10 – 12 July, 1995

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Introduction

The first Franco-British meeting on the physics and chemistry of the interstellar medium was held from 10 - 12 July 1995, in Lille. This meeting gave the UK participants the opportunity of travelling through the Channel Tunnel, perhaps for the first time. All participants experienced temperatures in excess of 35 C, at the start of what proved to be a long, hot summer in northern Europe. The meeting was sponsored by the Université Scientifique et Technique de Lille, the Région Nord Pas de Calais, The British Council, CERLA, the CNRS and PPARC.

The local organizers had been intending to provide hotel and restaurant facilities on the Villeneuve d'Ascq campus, where the meeting was held. The financial failure of the hotel-restaurant complex during the run-up to the meeting rendered this solution unworkable and gave the local organizers a lot of headaches. We are indebted to them for the initiative that they displayed in making alternative arrangements.

The meeting itself attracted over a hundred participants. Predictably, the largest contingent was French, and, fortunately, nationalities other than French and British did not feel excluded by the title. It was and still is intended that future meetings will more directly involve participants from other EU nations in their preparation.

Scientifically, the meeting was very successful, as the following summaries of the oral papers will testify. There was a substantial number of poster contributions, and these are being made available in the form of a supplement to this Newsletter. Our thanks are due to Simon Jeffery, secretary to CCP7, for his efforts in preparing the Newsletter and its supplement.

David Flower (Chairman, CCP7)

Observations of Molecular Outflows

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A review was given of the properties of molecular outflows in regions of star formation. I discussed briefly the history of the discovery of outflows and of their bipolar nature. I then considered their properties and showed examples of the contrasts between the morphology of the flows as seen in CO and that seen in the optical jets and HH objects. I also outlined current views on the forces driving the flows. The required momentum input is sensitive to estimates of flow lifetimes and I discussed the differences between dynamical ages and ages based on the statistics of outflows in molecular clouds. It seems likely that the momentum input from the observed optical jets suffices to maintain the CO flows.

The most recent development however is the discovery that some young (low luminosity) infrared sources in molecular clouds are associated with molecular flows which are more collimated and have higher velocities (by up to an order of magnitude) than the flows typically found in surveys. The infrared sources associated with such fast flows have extremely cold (20-30 K) spectral energy distributions and it appears that one may be observing an early phase in the development both of the flow and of the embedded source. One also finds chemical "anomalies" associated with the swept–up high velocity gas suggestive of the passage through a shock. These abundance differences include enhancements in methanol, SiO, and ammonia. There are similarities with the abundance distribution found in so–called hot core sources in regions such as Orion-KL . In this latter case, one believes that one is observing material that has been recently evaporated from icy grain mantles. A possible interpretation of the outflow anomalies is that we are observing the products of chemical processing on grain mantles which have been ejected into the gas phase due to sputtering within a shock.

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C I/CO observations in massive molecular cloud cores

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To determine the distribution of C° within interstellar molecular clouds is important for interstellar chemistry, since the C°/CO ratio is an essential chemical diagnostic. Although simple chemical models of PDRs predict that C°/CO becomes very small at high A_V, the distribution of C° is apparently very widespread. A popular explanation allows enhanced UV penetration into the clouds, if they are highly clumped. More refined models, including the disturbing effects of turbulent mixing and gravitational contraction, are appearing, and it is important to acquire observational data against which theoretical models can be compared.

We have recently made extensive measurements of $^3P_1 \rightarrow {}^3P_0$ 492 GHz CI line emission in the massive molecular clouds G34.3+0.2 and G35.2–0.74, using the James Clerk Maxwell Telescope. For these clouds we have measured C° and $C^{18}O$ distributions which can be compared with expectation based on the known UV illumination.

G34.3+0.2 has a relatively spherically symmetric structure, with a strong central condensation. Detailed radiative transfer modelling of its line shapes, as observed in emission from 492 GHz C°, and from ^{13}CO and $C^{18}O$ in several different rotational transitions, and assuming spherical symmetry, leads to a neutral hydrogen density varying as r^{-2}, and to a C°/CO ratio varying as $r^{0.9}$, from the perimeter of the cloud (at 3.5 pc) into r=0.24 pc where A_V=55 (Little et al. 1994, MNRAS, 271,649). The C°/CO ratio declines from about 0.4 at 3.25 pc to 0.04 at 0.24 pc. A steady, rather than an abrupt, decrease better fits the observations. The column density averaged C°/CO ratio is very similar to that for the ρ-Ophiuchi molecular cloud, notwithstanding its very different structure. Models for producing high C° deep in clouds which may have difficulty in explaining the similarity include those with external UV penetration around clumps, dynamic mixing, or in which the initial C°/CO >1.

G35.2–0.74 is probably the best example of an interstellar molecular disc which is definitely rotating. The disc, which is viewed edge on, has a dense inner core (diameter 0.4 pc). At the centre of the disc is an O/B star responsible for driving a CO outflow. While the CO outflow is very closely perpendicular to the plane of the disc, the alignment of the bipolar infrared and ionised hydrogen radiation is observed at increasing inclinations (up to 45°) to this perpendicular. It is likely that stellar wind jets emitted in opposite directions impinge on the biconical cavities they have excavated and ionise the N and S HII lobes by shock excitation. A precession of the jets could drive the observed CO outflow perpendicular to the disc.

Several components of the C° emission can be identified:

(i) background emission from the disc

(ii) an unresolved component from the central core

(iii) a low velocity tongue, aligned with the bipolar infrared nebula

(iv) a high velocity tongue aligned at an inclination between that of the bipolar infrared nebula and the CO outflow.

The column density ratios N(C°)/N(CO) at representative positions for these components, assuming a CO/$C^{18}O$ ratio of 500, are of order 0.05 to 0.10, except for the high velocity C° tongue where N(C°)/N(CO)=0.5 (Little & Kelly 1995, in preparation). The difficulty of isolating different components contributing to the column density along the line of sight needs to be stressed, however. The ratio in the low velocity tongue, in particular, could easily be much higher.

The observations support the model of the source in which a pair of oppositely-directed, ionized jets somehow transmit their momentum to the surrounding ambient medium, to produce the molecular outflow. The jets excavate a bipolar cavity which precesses with them, being filled in after the jets have moved on, and recreated in their new vicinity. Far-UV penetration along the cavity ensures that the C° abundance is high near its walls. CO forms in the outflow after the cavity has moved on, as the gas there is no longer illuminated with UV, and the C°/CO ratio falls to a few per cent.

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Recent observations of transient species in the laboratory: carbon and silicon compounds

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Many interstellar and circumstellar observed spectra remain unidentified:

- Some of the well known DIB's (Diffuse Interstellar Bands) were observed more than 50 years ago. Now, 200 bands have been detected in the visible and in the near infrared ranges but their carriers remain unknown;
- Concerning the more recently observed UIR (Unidentified InfraRed) bands, the choice between PAHs (PolyAromatic Hydrocarbons) and HACs (Hydrogenated Amorphous Carbons) is not definitively closed, even if very nice results related to different sorts of coal were presented at this conference;
- In the domain of radioastronomy, roughly 20% of the observed interstellar and circumstellar transitions are unidentified (see for example the compilation of F.J. Lovas "Recommended rest frequencies for observed interstellar microwave transitions–1991 revision" appeared in J. Phys. Chem. Ref. Data, 21, 181–272, 1992).

The final identification of all these observations needs their detection in the laboratory, "the last court of appeal" (P. Thaddeus, AIP Conference Proceedings 312, "Molecules and grains in space", ed. I. Nenner, New York, p. 711–731, 1994), but what can help the spectroscopist in the choice of new interesting molecules from the interstellar point of view?

Different possible cases are illustrated:

- Unidentified spectrum observed by radioastronomy with different hypothesis on the identification like $HOCO^+$ from Thaddeus et al. Astrophys.J. 246, L41, 1981, or $MgNC$ from the observation of Guelin et al. Astron. Astrophys. 157, L17, 1986;
- "Chemical intuition" which leads the spectroscopist to the choice of possible candidates for astronomical search. For example, $HCOOH$, $HCOCH_3$, $HCONH_2$, $HCOCCH$ are equivalent to formaldehyde through the substitution of an H atom by respectively the OH, CH_3, NH_2, CCH radicals and all these compounds were detected in the interstellar medium: then, $HCOCN$, obtained through the substitution of H by CN seems to be a good candidate;
- Classification of the molecules identified in the interstellar and circumstellar media in series and research for missing elements of these series: C_nH known up to C_6H, $HC_{2n+1}N$ observed up to $HC_{11}N$, carbon clusters: C_2, C_3 and C_5 have been detected...
- Many silicon equivalent of carbon compounds have been observed and some new ones can be searched for: SiO, SiC, SiC_2, SiC_4... have been observed but $HNSi$ was never detected due to a weak dipole moment.

In the last years we observed in our laboratory different molecules corresponding to silicon equivalents of carbon compounds: isotopic substitutions of SiC and SiC_2, SiC_2 in the ν_3 vibrationally excited state, $HNSi$, Si_2H_2 and H_2SiO, and a molecular ion, protonated acetylene $C_2H_3^+$. Only the most recent results concerning H_2SiO and $C_2H_3^+$ will be developed. During that time, the group of Saykally in Berkeley, California, obtained very interesting results by infrared and far infrared spectroscopy on carbon clusters.

Formaldehyde is an important ubiquitous molecule in the interstellar medium. So, we started a search for its silicon equivalent H_2SiO. In order to synthesize this compound, we tried first fash thermolysis experiments which led only to SiO, and then, electric discharge in a mixture of SiH_4, O_2 and Ar. A large number of lines were detected belonging all to short-lived species. The observed spectrum was so dense that we were unable to identify some typical pattern. In order to discriminate the lines, we measured their lifetimes by using a square-wave modulation of the discharge. Different lifetimes were measured and the lines corresponding to the shortest one were easily ascribed to H_2SiO. The observation of different isotopic substitutions ^{29}Si, ^{30}Si, ^{18}O and D_2, led to a precise determination of the molecular structure. Nevertheless, this molecule has not been detected by radioastronomy until now.

Concerning $C_2H_3^+$, the abundance of this ion in the interstellar medium was predicted high enough by chemical modelling calculations in order to allow its observation. From the spectroscopic point of view, only one infrared band was known and did not allow the determination of the A rotational constant which is absolutely required to predict the millimeter-wave spectrum. Then, we started a search for this spectrum in a plasma of C_2H_2, H_2 and Ar. Seventeen lines were identified and the determination of the molecular constants has allowed the prediction of all the millimeter-wave spectrum. The most interesting transitions for radioastronomy were blended by atmospheric lines. Nevertheless, a search were carried out with the IRAM radiotelescope and at Hawaï. It was unsuccessfull and the highest limit of the abundance which was obtained did not agree with the theoretical predictions.

Up to now, three carbon clusters have been observed in the interstellar and circumstellar media: C_2, C_3 and C_5. Experimental results on other clusters are requested in order to allow their search by infrared and far-infrared astronomy. The group of Saykally (Berkeley, California) has obtained very interesting results on these compounds by a laser ablation experiment in a supersonic beam. Many clusters have been observed like C_3, C_4, C_5, C_6, C_7, C_9 and C_{13} but always in their linear structure even if ab initio calculations predict a non-linear lowest energy structure for the largest clusters. The predicted alternation between singlet Σ and doublet Σ ground state, respectively for the odd and even number of atoms (except for C_2), has been observed.

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Gas-phase syntheses of potential interstellar molecules

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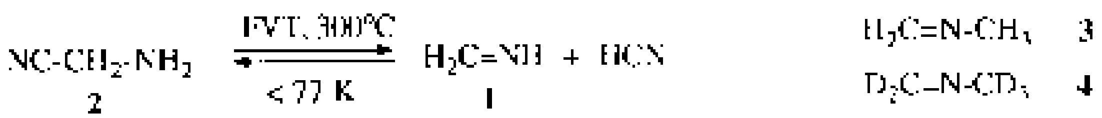
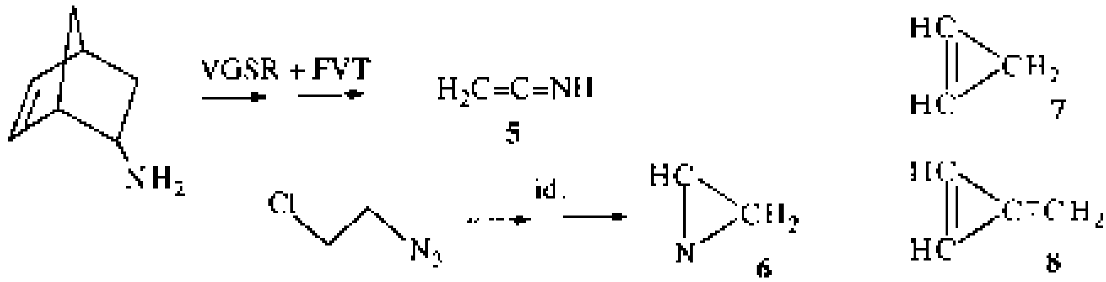
Flash vacuum thermolysis (FVT) and vacuum gas-solid reactions (VGSR), developed in our groups, are particularly suitable methods for accessing in the gas-phase extremely reactive species. FVT is a dynamical gas-phase thermolysis operating under high temperature and vacuum, and avoiding mostly any intermolecular and catalytic pathways. VGSR involves the reaction under vacuum between a gaseous precursor and a solid reagent. It requires moderate temperature and, unlike FVT, allows to generate unstable, strained species. Both methods thus complete each other perfectly and can also be used jointly on the same vacuum line. Under the auspices of the GDR PCMGI, we have undertaken to generate in that way several kinds of heteroatomic, reactive molecules postulated as possible interstellar species. After perfecting the conditions of reaction, the short-path coupling of FVT or VGSR with an especially designed millimeter wave (MW) spectrometer, realized at the Laboratoire de Spectroscopie Hertzienne (URA CNRS 249, Lille), has allowed to determine the MW spectra of these molecules.

Nitrogen compounds:

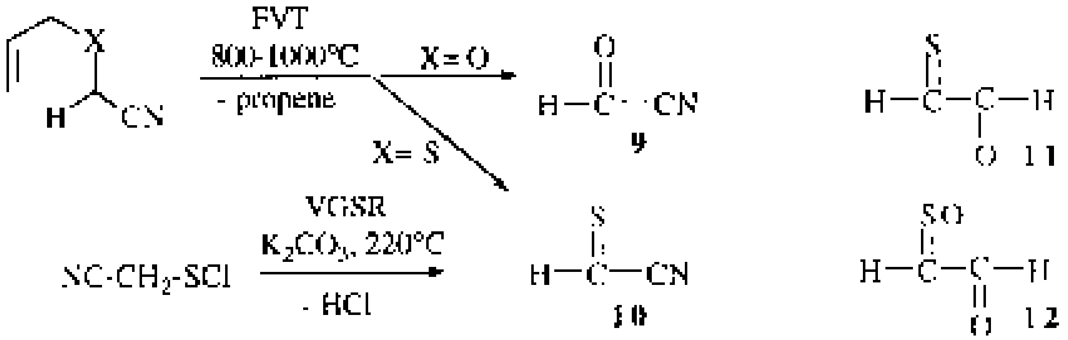
Methanimine (1) has been generated from several precursors, either by VGSR or FVT, and in best conditions by FVT of aminoacetonitrile (2). The recombination of 1 with hydrogen cyanide at very low temperature suggests the possibility of this reaction and the presence of the prebiotic molecule 2 in the IS medium. The MW spectra of 2, and of the similarly obtained methanimines 3 and 4, have been thus determined.



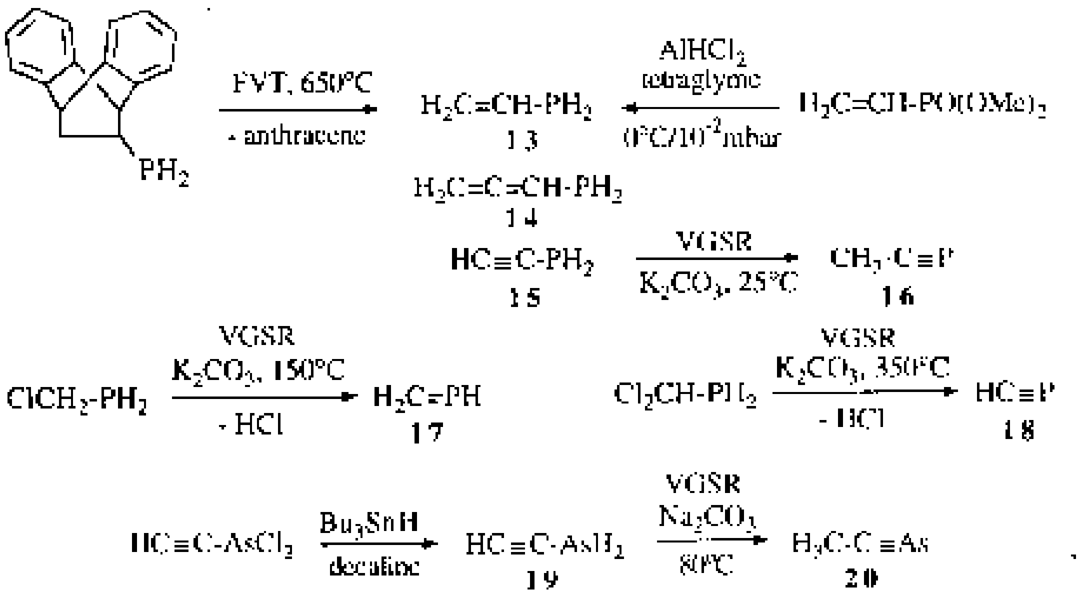
Ketenimine (5) and Δ^1-azirine (6) have been obtained using on the same vacuum line VGSR and FVT reactions. TheVGSR of halogenocyclopropanes led also to the small ring molecules 7 and 8. The MW spectra of compounds 6-8 have been recorded.



Oxygen and sulfur compounds:
Retro-ene reactions using FVT led to generate and determine the MW spectra of formyl cyanide (9) and thioformyl cyanide (10), this latter being also obtained by VGSR. The related species thioxoethanal (11) and its S-oxide 12 have been similarly synthesized by FVT.



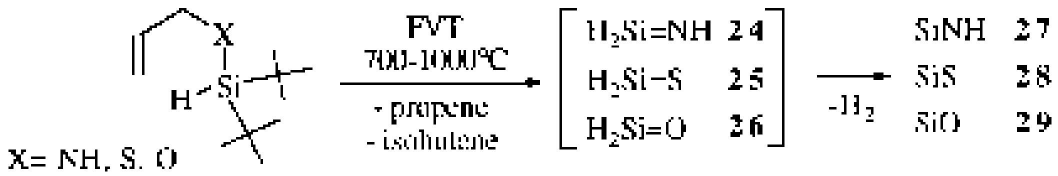
Phosphorus and arsenic compounds:
Vinyl phosphine (13) has been generated by FVT (retro-Diels-Alder reaction) as well as by direct reduction of the corresponding phosphonate, under vacuum in a high-boiling solvent. The latter reaction led also to allenyl and ethynylphosphines (14 and 15). The MW spectrum of 13 has been investigated. The action of potassium carbonate under VGSR conditions transformed 15 into phosphapropyne (16). Phosphaethylene (17) and phosphaacetylene (18) have been generated by VGSR. Related reactions led to generate ethynylarsine (19) as well as arsapropyne (20) and all its ^{1}3C and ^{2}H isotopes, these latter being investigated in detail by MWS.



Silicon compounds:
The investigation of double-bonded silicon species has been undertaken. Unhindered silanimines such as 21 have been characterized as monomers in the gas-phase. The N- unsubstituted silanimine 22 and the silathione 23 have been also unambiguously generated. However, the parent silanimine (24), silathione (25) and silanone (26) could not be obtained by FVT, owing to the dehydrogenation on silicon leading respectively to silaisonitrile,

silicon monosulfide and silicon monoxide (27-29), characterized by MWS.

$(H_3C)_2Si{=}N{-}CH(CH_3)_2$ **21** $\quad$ $(H_3C)_2Si{=}NH$ **22** $\quad$ $(H_3C)_2Si{=}S$ **23**



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Laboratory investigations of interstellar medium constituents: the ion trap technique.

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When devising laboratory experiments to study the physical and chemical properties of the interstellar medium constituents, the major problem encountered comes from the difficulty to mimic the extreme environment conditions, especially the very low density. The ion trap, which provides an environment free of collisions during long periods, is a good answer to this problem. Although limited to studies concerning charged species or charged-neutral reactions, this device can provide information that cannot be obtained by the other commonly used techniques, matrix isolation and supersonic jets. Among the different methods of ion confinement, magnetic traps of the Penning type (Ionic Cyclotronic Resonance -ICR- cells) are of special interest. They provide the longest trapping times (up to hours) and offer the possibility of *in-situ* non destructive analysis of the ion cloud composition by Fourier Transform Mass Spectroscopy (FT/MS).

With their ability to store large molecular ions, these devices are well suited to the study of Polycyclic Aromatic Hydrocarbons (PAHs) and related species, which are supposed to be abundant in the ISM. Several results of astrophysical importance have been recently obtained, in our laboratory (poster P. de Parseval *et. al.*) as well as in other groups. These results will be presented and their astrophysical implications will be discussed.

More recently, the formation and the reactivity of organometallic complexes between PAHs and transition metals have been investigated. The possible existence of such complexes in the ISM has been recently proposed (G. Serra *et. al.*, A&A. **260**, 489, 1992). Our experimental results confirm their stability (P. Boissel, A&A. **285**, L33, 1994) and demonstrate the role that they could play in the ISM chemistry (poster P. Marty *et. al.*).

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Laboratory Measurements on Important Astrophysical Reactions between Neutral Species

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Until very recently there had been virtually no kinetic data for bimolecular reactions between electrically neutral species at temperatures below *ca.* 200 K. Guided by the fact that the rate coefficients for many such reaction exhibit a marked positive dependence on temperature, whereas those for many ion-molecule reactions are known to stay constant or increase as the temperature falls, chemical models of interstellar clouds (ISCs) have tended to ignore the former and empasise the latter. However, the fundamental requirements for a positive temperature-dependence, the existence of a potential energy barrier for the reaction is not satisfied by some classes of neutral-neutral reactions - most notably those between free radicals, such as $O(^3P)+OH(^2\Pi) \rightarrow (HO_2) \rightarrow O_2+H$, which proceed through a transient complex. Recognising this, some models have assumed that the rate coefficients vary with temperature according to the simple model of collisions between 'hard-spheres' for which the rate coefficient varies as $T^{1/2}$.

Two sets of experiments have, in recent years, explored the variation of rate coefficients, k(T), with temperature for neutral-neutral reactions below 200 K.[1] They and the results of the measurements are reviewed briefly in this paper. Both groups of experiments employ the well-established PLP-LIF technique. A particular radical is generated by pulsed laser photolysis (PLP) of a suitable precursor (*e.g.*, CN radicals from NCNO). The subsequent kinetics of that radical is observed by tuning a laser to a line in its electronic spectrum, thereby obtaining laser-induced fluorescence (LIF) signals whose intensity reflects the concentration of the radical at the instant when the probe laser is fired. By varying the delay time between pairs of laser pulses one obtains a complete kinetic history of the radical.

The PLP-LIF method has been complemented in two different environments. The more conventional experimental arrangement, which accesses temperatures down to *ca.* 80 K,[2] employs cryogenic cooling of a gas mixture flowing through the reaction cell at a speed which is slow enough to prevent condensibles (such as the radical precursor) from entirely freezing out on the walls of the reactor. The more novel approach, yielding much lower temperatures (<< 80 K), is to implement the PLP-LIF method in a gas mixture which has been cooled by expansion through a Laval nozzle in a CRESU apparatus.[3] As is shown below, the two techniques are complementary: the cooled cells cannot access the extremely low temperatures available in the CRESU apparatus but they do allow rate measurements on some sytems that cannot - at least, as yet - be studied in a CRESU apparatus.

Already the CRESU apparatus in Rennes has provided rate data for a range of reactions and energy transfer processes involving CN,[3,4] OH,[5-7] CH(v=0)[8] and CH(v=1)[8] radicals with saturated molecules, unsaturated molecules and free radicals. To illustrate the variety of temperature-dependences that the rate constants display, I refer here to three examples: (1) $CN + O_2 \rightarrow$ products; (2) $CN + C_2H_2 \rightarrow C_2HCN + H$; and (3) $CN + C_2H_6 \rightarrow C_2H_5CN + H$.

Reaction (1) was the first reaction which was studied at both low and ultra-low temperatures.3 It is clear that O_2 acts as a radical so that reaction proceeds by way of an NCOO transient species accessed by means of monotonically attractive potential between the reagents. The rate constants vary with temperature according to the expression $k(T) = 2.5 \times 10^{-11}(T/298)^{-0.63}$, with some evidence that they may reach a saturation value below 25 K. These results are consistent with adiabatic capture on an attractive surface being rate-determining and with 'tightening' of the transition state region as the temperature is raised.

Reactions of CN and C_2H with alkynes may be responsible for the formation of cyano-poly-ynes in ISCs. The rate constants for reaction (2) increase in value down to *ca.* 100 K and then remain constant, or possibly decrease slightly, as the temperature is lowered further. The values at and below 100 K are consistent with capture by the long-range intermolecular potential arising from dispersion and induction forces. These forces are stronger in the case of $CN + C_2H_2$ than for $CN + O_2$, so the limiting value of the rate constant is reached at higher temperatures.

The most surprising results obtained so far are those for $CN + C_6H_6$. Here, the rate constants show a positive temperature dependence above 300 K but pass through a minimum at ca . 150 K and rise as the temperature is lowered further. This complex behaviour must reflect subtle changes in the transition states for reaction as the temperature - and hence the collision energies and rotational state populations change.

Experiments in cryogenically cooled cells not only provide an important check on those in the CRESU apparatus. They also allow measurements (a) at higher total pressures, *e.g.* for the reaction of CH with H_2,[8] (b) on slower reactions, *e.g.* on that between OH and CO;[2] and (c) on reactions between pairs of unstable species, *e.g.* those between OH and N and O atoms.[9] In the context of the chemistry in ISCs, all of these measurements are useful, but the last may be especially valuable since many of the neutral-neutral reactions which may be important in ISCs involve pairs of unstable radicals.

Our measurements clearly demonstrate that the role of neutral-neutral reactions in the chemistry of ISCs has been underestimated. Unfortunately, there is no straightforward way to predict the rate constants for such reactions at temperatures below 50 K, although reasonable estimates for radical-radical reactions and for reactions between radicals and unsaturated molecules may be made via a simple capture approach making due allowance for the effects of electronic degeneracies and near degeneracies in the reagent species.[10] Future targets for kinetic measurements at ultra-low temperatures in the CRESU apparatus in Rennes and the new apparatus in Birmingham include reactions of C atoms and of C_2H radicals both of which are likely to play important roles in the chemistry of ISCs.

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Fast-flow studies of N + CH → CN + H and N + C_2 → CN + C neutral reactions.

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The N + CH → CN + H and N + C_2 → CN + C neutral reactions are believed to play a key role for the production of CN radical in diffuse and dense dark clouds of interstellar medium[1]. An ab-initio study of the two potential energy surfaces involved for the reaction N + CH → CN + H has shown that one of these surfaces has no potential energy barrier while the other possesses a very small one. Soon later, this theoretical result was confirmed by an experimental determination of the rate constant value which was found to be nearly gas kinetic at room temperature, i.e. $2*10^{-10}$ cm^3 $molecule^{-1}s^{-1}$, and unsensitive to a temperature decrease[2]. To our knowledge, neither theoretical nor experimental studies have been performed for the reaction N + C_2. Such reactions proceed through the more or less "long-lived" complexes HCN and NC_2 owing to the deep potential energy well between the reactants and the products. The rate constant value which is capital for kinetic modeling, allows to appreciate the barrier effect but cannot give an information related to the whole potential energy surface from the reactants to the products. Such an information is given by the reaction dynamics. In particular, J.C. Rayez and coworkers, using models of potential energy surfaces involving a well, found that the depth of the well is of minor importance. The dynamics is governed by the anisotropy of the well[3]. For a well corresponding to a linear triatomic configuration ABC, the anisotropy factor is defined as the ratio ρ of quadratic forces constants k_{AB} and k_{BC} at the potential energy minimum along the AB and BC directions. It has been shown that this factor is directly related to f_v, the fraction of energy available to the products which is channeled into the vibration of the diatomic product. The more ρ departs from 1, the greatest the value of f_v. These two reactions offered the opportunity to check these conclusions. The well corresponding to HCN is likely to be more anisotropic than the well corresponding to NC_2. A greater vibrational excitation of CN is thus expected with the reaction N + CH than with the reaction N + C_2.

These reactions have been studied in a fast-flow reactor with reactants diluted in He at a pressure of 0.5-2 Torr. CH and C_2 radicals were obtained from $CHBr_3$ and C_2Cl_4 by successive strippings of halogen atoms by K atoms. The CN radical was probed by laser-induced fluorescence. To get a stationary vapor pressure of potassium close to 1 mTorr, solid potassium was heated at 473 K so that the reaction in the flow tube occured at 429 K as determined by the rotational temperature of CN.

The exoergicities of these reactions, taken as the energy difference between the zero-point levels of reactants and products, are respectively of 4.30 $\pm$ 0.05 eV and 1.48 $\pm$ 0.07 eV. The first electronically excited state of C_2, $a^3\Pi_u$, is just 0.089 eV above the ground state $X^1\Sigma_g^+$ so that at 429 K it amounts to 35 % of the total C_2. The mean thermal (translational and rotational) energy of the reactants is $\frac{5}{2}kT$, i.e. 0.09 eV. The mean thermal energy available to the products is then 4.39 $\pm$ 0.05 eV for the N + CH reaction, 1.57 $\pm$ 0.07 eV for the N + C_2 ($X^1\Sigma_g^+$) reaction and 1.66 $\pm$ 0.07 eV for the N + C_2 ($a^3\Pi_u$) reaction. The N + CH and the N + C_2 reactions thus allow to populate CN in its electronic ground state respectively up to v"=19 and v"=6 vibrational levels. The first reaction leads to a vibrational population inversion with a maximum population at v"=4 while the second gives a decreasing, near-statistical, vibrational distribution but which exhibits a small peak at v"=4. The statistical distribution is given by the probability P^o(v) which can be expressed as a function of f_v, For a rigid rotor-harmonic oscillator, it is given by the expression : $P^o(v) = \frac{5}{2}(1 - f_v)^{\frac{3}{2}}$. The distribution from N + C_2 reaction is very similar to that obtained in crossed beams from the C + NO $\rightarrow$ CN + O reaction at a total energy available to the products of 1.50 eV[4].

Theoretical calculations had determined an isotropic potential energy well for the C + NO $\rightarrow$ CN + O reaction and trajectories on the potential energy surface found that small peak. These vibrational distributions are consistent with theoretical predictions for three-atom reactions involving a potential-energy well.

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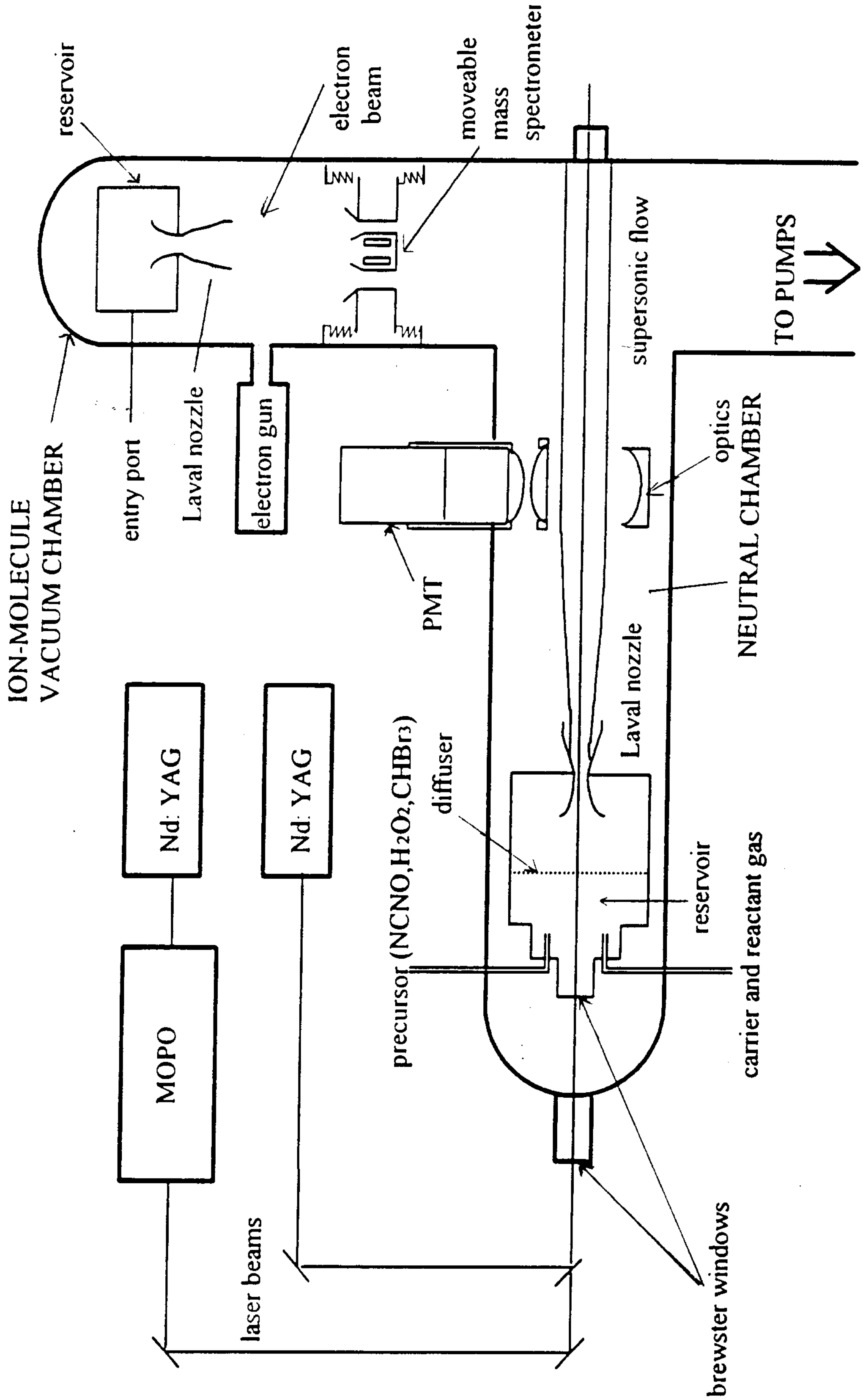

Figure 1. (Canosa et al.) The CRESU apparatus at the University of Rennes.

The CRESU apparatus at the University of Rennes

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The CRESU apparatus (French acronym for "Cinétique de Reaction en Ecoulement Supersonique Uniforme" which means Kinetics of Reaction in Uniform Supersonic Flow) was firstly developed by Rowe and coworkers in the early eighties at the laboratoire d'Aerothermique in Meudon (France) [1]. Recently a new CRESU has been built at the University of Rennes. It is devoted to the study of chemical reactions at very low temperature (13-300 K) and in the gas phase. The apparatus is operational since 1992 and has been initially dedicated to the study of radical-molecule reactions [2-7]. Since October 1994, a second chamber (see figure 1) has been available for the study of ion-molecule reactions [8].

The apparatus will be presented in detail at the conference as well as the results tht were obtained in the field of both radical-molecule and ion-molecule reactions.

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Vibrationally excited H_2 molecules desorbed from carbon surfaces

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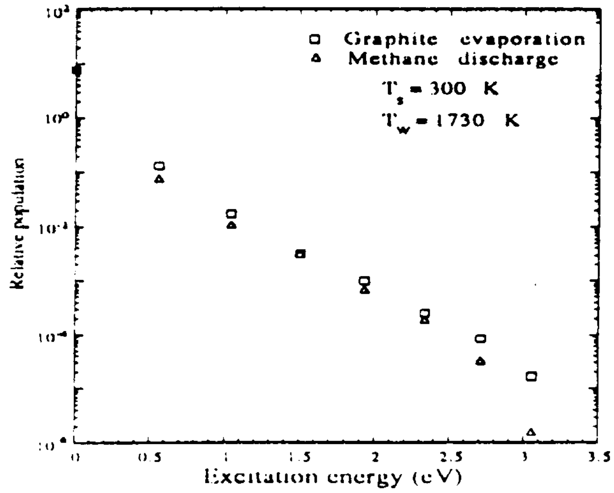
We have shown, in the laboratory, that recombination of atomic hydrogen from carbon surfaces can produce strong vibrational excitation of the molecules formed [1]. This observation has been done with pure carbon and hydrogenated carbon surfaces, for surface temperatures varying from 300 K down to 90 K. The reaction occurs in a cell containing about 10^{15} molecules and 10^{13} atoms per cm^3, namely upon high coverage surfaces.

The carbon surface is prepared *in situ* after wall cleaning by argon discharge. The inner surface of the cell is coated with a layer of carbon using one of two methods. In the first, a graphite filament is evaporated onto the cell wall giving a fine, but irregular, polycrystalline carbon surface. In the second method, carbon is deposited by striking a discharge of 100 mA in methane at 0.25 Torr for 30 minutes. This gives a much thicker polycrystalline surface with crystal sizes of up to 10μm.

The experimental cell comprises a stainless steel cylinder surrounded by a cooling jacket. By controlling the nature and the flow rate of the cooling fluid the cell wall temperature may be precisely controlled. A tungsten filament heated to 1800 K produces atomic hydrogen by thermodissociation of molecular hydrogen. During the experiment, molecules formed by recombination on the carbon surface, as well as atoms and undissociated (v=0) molecules, effuse from the cell and are crossed by a low energy and high resolution electron beam. The detection method [2] of vibrationally excited molecules is based on the dissociative attachment (DA) process:

$$e + H_2(v) \rightarrow H_2^- \rightarrow H^- + H$$

The H^- ions formed in this process are detected. Sweeping the incident electron energy from 4 to 0 eV produces a peak in the measured H^- signal at the threshold for DA from each vibrational level of H_2. Since the dissociative attachment cross-sections are well known, the peak heights allow us to determine the corresponding level populations



The populations obtained at 300 K for the two surfaces, are displayed in the figure. At 90 K the populations are lower, but the ratio between v=1 and v=0 is still estimated to be between 2.5 and 7%.

The study of the stabilization time of the spectra seems to indicate that the formation for low and high levels are based on different mechanisms, as observed previously on metals [3].

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Recent interstellar models: how secure are the predictions?

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High resolution spectral observations have led to the unambiguous detection of over 100 gas-phase molecules in interstellar and circumstellar clouds, while low resolution observations have yielded much information about dust grains and very complex molecules. A variety of gas-phase and gas-grain chemical models have been developed to understand these observations and to predict the results of future observations. Yet these models are not totally secure because of chemical, physical, and astronomical uncertainties.

Perhaps the most secure result of gas-phase chemical models is the prediction that in the interiors of cool dense interstellar clouds, large abundances of CO will exist after a time of 10^{4-5} yr. Closer to the cloud edge but inside a layer of C^+, a large abundance of C is predicted, especially at times up to 10^6 yr. In addition to the CO prediction, gas-phase models predict abundances for large numbers of molecules in the interiors of dense clouds. The qualitative predictions concerning ions, metastable neutrals, isotopic fractionation, and severely unsaturated molecules are in agreement with observation, and suggest that ion-molecule reactions still dominate the gas-phase chemistry despite recent experiments that show selected neutral-neutral reactions to be quite rapid at low temperatures. Moreover, despite continuing uncertainties in the rates of key processes such as dissociative recombination, the calculated abundances for individual small molecules are generally in reasonable agreement with observed values for all times past 10^5 yr. For the larger molecules, calculated abundances are significant only at early times (10^5 yr) in simple one-phase approaches, although these large abundances can persist with more complex physical conditions. The calculated abundances of complex molecules are very sensitive to assumptions about the rates of neutral-neutral reactions. Gas-phase models have recently been extended to include unsaturated molecules as large as fullerenes.

The chemistry on dust surfaces is known to exist and to be diffusive in nature, yet the uncertainties are much larger than for gas-phase chemistry. Current gas-grain models predict that chemically saturated species such as ammonia, water, and methanol dominate the mantles of cold dust particles in dense interstellar clouds at most times. Observations show, however, that unsaturated species such as CO as well as unidentified non-polar species may be more important than models indicate. The rate equations used in these models have recently been questioned, and it may well be the case start here that the role of hydrogenation has been overestimated. Another continuing uncertainty in gas-grain models is the role and cause of non-thermal desorption.

In addition to cool, quiescent clouds, modellers have considered all sorts of more active sources related to star formation such as Hot Cores, photon-dominated regions, turbulent regions, and shocked regions. These distinctive regions have distinctive chemistries from cooler sources and from each other. Models for some of these sources are quite successful in interpreting what makes them distinctive, although in general the uncertainties are larger than for quiescent sources.

The interstellar medium in external galaxies

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INTRODUCTION

Despite the wealth of knowledge on the interstellar medium in The Milky Way, astronomers gain also advantage at studying interstellar processes in external galaxies. These objects offer a larger range of physical conditions with varying star formation activities and metallicities and thus enable to follow the status of the interstellar gas in abnormal conditions (from a Milky Way point of view).The dynamical processes are better enlightened and easily recognized in external galaxies whereas the spiral structure of the Milky Way is still debated. Therefore the external galaxies offer a complementory view of the most important physical processes for the study of the interstellar medium. I present in the next section the basic tools used to measure the gas content of external galaxies, then two types of research on galaxies and finally some perspectives for the future.

TOOLS AND UNCERTAINTIES

To observe the cold interstellar medium in galaxies, the astronomers use three basic tools. First of all, the main constituent of the interstellar gas mass is the neutral hydrogen, easily detected by its hyperfine transition at 21 cm. The only disadvantage of this reliable gas tracer is the very extended distribution of the neutral hydrogen, usually found beyond the optical disk. Carbon monoxyde, CO, has been observed since 25 years as a tracer of molecular hydrogen H_2. Because it is a symmetric molecule, the allowed ground state transitions of H_2 are extremely weak. By contrast CO is widespread in molecular clouds and its ground state rotational transitions at 2.6 mm (J=1-0) and 1.3mm (J=2-1) are easily detected. The measure of the molecular hydrogen mass from CO is much more uncertain than the measure of the neutral hydrogen mass : the H_2 mass is deduced from the CO emission through a conversion factor X estimated in the Milky Way. The constancy of this factor from galaxy to galaxy or even inside a given galaxy is assumed as a zero order approximation. However Sodroski et al (1995) have presented good evidences that X increases by a factor at least 3 between the Galactic Center and the solar vicinity. In low metallicity galaxies such as the Magellanic Clouds, X seems also to be larger than in the Milky Way (Rubio et al. 1993, Wilson 1995). Molecular gas masses ΞΞΞΞΞare nevertheknown within a factor two, for large spiral galaxies. Finally, with the advent of sensitive bolometers, it is possible to measure the thermal emission of the dust grains inside the interstellar clouds. This emission scales linearly with both the dust mass and the dust temperature. The interpretation is therefore easy, with the only caveat coming from the poor knowledge of the dust properties at millimeter wavelengths and the possibility of systematic variations of the dust properties inside a galaxy, or from galaxy to galaxy (dust is expected to be more abundant relative to the gas in metal rich galaxies). The very good agreement between the dust and CO maps at high resolution (Guélin et al 1993, 1995) on the one hand, and the good correlation of the dust and CO emission at a the global scale (Andreani et al 1995) on the other hand show that bolometer observations are a promising direction. The smooth spectrum of high latitude gas in the Milky Way, from the far infrared till the millimeter wavelengths, further supports the derivation of dust masses from the fluxes at 1 mm (F. Boulanger 1995). Using these tools, astronomers may take two different approachs to investigate the interstellar medium in galaxies, either focus on one particular galaxy as M51 or look for average properties in galaxy samples.

INDIVIDUAL GALAXIES : THE EXAMPLE OF M51

The beautiful spiral structure of this nearby galaxy has been fully mapped in CO(J=2-1) (Garcia-Burillo et al. 1993a) and shows up as well in CO as in the visible light. This highly contrasted CO map emphasizes the role of dynamical processes in organizing the stars and gas in the galactic disk. Garcia-Burillo et al (1993b) tested the ability of numerical models of the gas flow in spiral galaxies to reproduce the spiral pattern observed in M51. Using optical and near infrared images as inputs for a mass model, they succeeded to reproduce the observed molecular gas distribution : the interstellar medium is represented by an ensemble of gas clouds interacting through inelastic collisions (Combes and Gerin 1985). The stellar spiral structure creates a perturbing gravitational potential which forces the clouds to gather in the spiral arms. The validity of this approach is supported by the sensitivity of the model cloud distribution to the pattern speed of the spiral structure. This method has been applied to other spiral galaxies (e.g. Sempere et al . 1995), showing the importance of the density wave to organise the global distribution of the interstellar medium. The ability to model so well the gas distribution is a good support for the presence of stable density waves (modes) in spiral galaxies, both in the gaseous and in the stellar components.

GALAXY SURVEYS

To investigate further the relations between gas content, star formation rate and morphological type, it is necessary to use a statistical approach. The first and dominant effect seen in large galaxy samples is known as the size effect : the bigger the galaxy, the larger its gas mass or luminosity at any wavelength. Therefore, it is better to use hybrid surface densities or surface brightness to characterize galaxy properties independently of their sizes. The best relationship is found between the H_2 surface density (deduced from CO) and the far infrared luminosity (FIR). This nearly linear relationship can be used as a good predictor for the CO flux of a galaxy, in addition to its size (Andreani et al. 1995, Sauty et al. 1995). There is in contrary no correlation at all between the neutral and molecular hydrogen surface densities. But the most striking result of these galaxy surveys is the relative lack of molecular gas. The H_2 surface density is nearly constant among spiral types but amounts to 20 percents only of the surface density of atomic hydrogen . CO rich galaxies like M51 are quite rare, and are found mostly among far infrared luminous galaxies. The common view that star formation is related to the amount of molecular gas seems then oversimplified : infall and conversion of HI to H_2, cloud destruction by massive stars and variation of the CO to H_2 conversion factor blurr this picture. Surveys with a large number of galaxies should be able to shed more light on this question in the near future.

PERSPECTIVES

With the increased sensitivity of detectors, it is now possible to observe galaxies at cosmological distances. If most of the currently detected objects are amplified by gravitational lenses, this bias should become less important with the advent of larger telescopes and even more sensitive receivers. Furthermore the launch of ISO will further open the infrared window : the strongest cooling lines of the interstellar medium, the C^+ line at 158 μm and the O line at 61 μm, will be observed in a large galaxy sample hence providing a new look at the global energetic budget of galaxies. On the other side of the infrared window, the near infrared cameras offer a new way to take images of galaxies. Without the screening effect of the dust, the spiral disks appear smoother with a clearly defined structure (Block et al 1994). With a narrow band filter, it is possible to select one emission line and thus to map strong emission lines of the ISM at very good spatial resolution. Such images are particularly interesting because of the huge jump in spatial resolution between the structures observed in our Galaxy and those observed in external galaxies : with a pixel size of 1 arcsec, which can be achieved at visible as well as at radio wavelengths, the linear resoluion jumps from 0.002 pc in the nearby Orion molecular complex (at a distance of 450 pc) to 48 pc in the galaxy M51 (distance of 10 Mpc) and to 200 pc in Arp299 (distance of 41 Mpc). Therefore, lots of effort are still required to interprete properly the current observations of external galaxies. This is a new challenge for the research on the interstellar medium outside the Milky Way.

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Organometallic contribution to the interstellar depletion

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Associative collisions are efficient between ionized metals and aromatic molecules (e.g. see the poster of Marty et al.). If organometallic complexes exist in the diffuse interstellar medium (ISM) they must be taken into account in the depletion processes.

We performed ab-initio calculations (generally at MP2 level) for complexes $[M(benzene)]^+$ where M = Li, Na, Mg, Al, Si, K, Ca and Zn. Geometries of complexes were fully optimized and bonding energies between metals and benzene were computed. Other bonding energies were found in the literature for M = Ti, Cr, Mn, Fe, Cu, Ni. These data allowed us to find a good correlation between the ISM depletion and the bonding energies of metals with benzene. Such a correlation should not be dramatically different for polycyclic aromatic hydrocarbons (PAH). This correlation means that, the more a metal is bonded to a PAH, the more it is depleted in the gaz phase of the ISM.

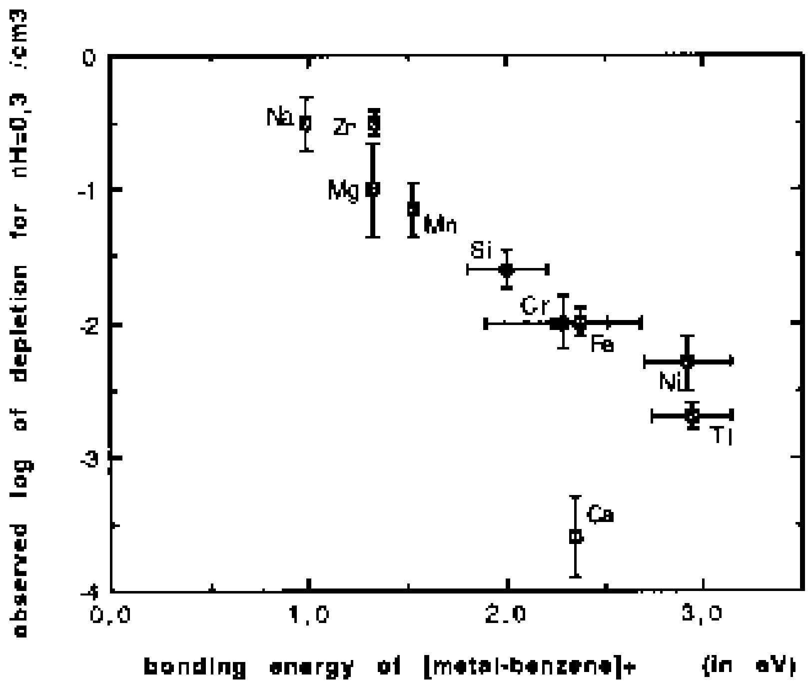

Fig.1. Correlation between the bonding energy of $[M\text{-benzene}]^+$ molecules and the depletion of metals in a low irradiated medium ($n_H \sim 0.3\mathrm{cm}^{-3}$).

A simple modeling of three components : gas / grains / organometallics was applied in the diffuse ISM (Klotz et al. 1995, A&A accepted). We deduced that organometallic complexes should contribute from 5% to 10% of the metal depletion in ISM. This modeling, based on the thermo-photo-dissociation processes of the $[M(PAH)]^+$ complexes, led us to constrain the distribution law of the size of PAHs. We found a law of distribution which exhibits a $1/C^2$ dependence (C is the number of carbons in the PAH). This dependence is the same as that of the modeling of Désert et al. (1990, A&A 237). Moreover, our modeling predicts the existence of large complexes that contain more than 1000 atoms. It is possible that this complexes are constituated by small PAHs bonded each others by metals. So, organometallics in the ISM could be the link between PAHs and Very Small Grains (VSG).

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Diffuse Interstellar Bands and Large Carbon Molecules

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Astronomical observations revealed up to now 150 diffuse interstellar bands (DIBs) at wavelengths ranging from the blue part of the visible spectrum to the near infrared (Herbig 1975, Herbig & Leka, 1991, Jenniskens & Désert 1994). Current high S/N observations do reveal more and more weak DIBs. Several possible carriers of solid state origin and gas phase molecules have been proposed (see for a review: Smith et al. 1977, van der Zwet 1987). Though the carrier molecules are still not identified, new results indicate that some of the carriers of the DIBs may be families of molecules based on carbon, which are ubiquitously present in the interstellar medium.

Polycyclic aromatic hydrocarbons (PAHs), fullerenes and their ions were reported as promising candidates (Leger & Puget 1984). Recently, laboratory measurements using rare gas matrices have provided a set of spectra of PAHs and PAH ions which allow a good comparison with interstellar data and show that small PAHs may account for several DIBs (Salama & Allamandola 1992a,b). Large ionized carbon molecules show strong transitions in the near infrared, a rather unexplored spectral region for astronomy. We have searched in particular for new DIBs above 9000 Å in order to identify $C_{60}{}^+$, the coronene and ovalene cations in the diffuse interstellar medium. Observations have been performed with the 1.52 m Coude telescope/spectrograph Aurelie (at OHP, Observatoire Haute Provence) with a spectral resolving power R=36.000.

The detection of two new diffuse bands that are coincident with laboratory measurements on $C_{60}{}^+$ in a Neon matrix have been recently reported (Foing & Ehrenfreund 1994). ¿From these observations and the total absorption, we estimate that up to 0.9 % of interstellar carbon may be in the form of $C_{60}{}^+$, which indicates that fullerenes may play an important role in interstellar chemistry. These results provide strong evidence for the existence of the C_{60} cation as the largest molecule ever detected in space and likely represent the first direct identification of diffuse interstellar bands.

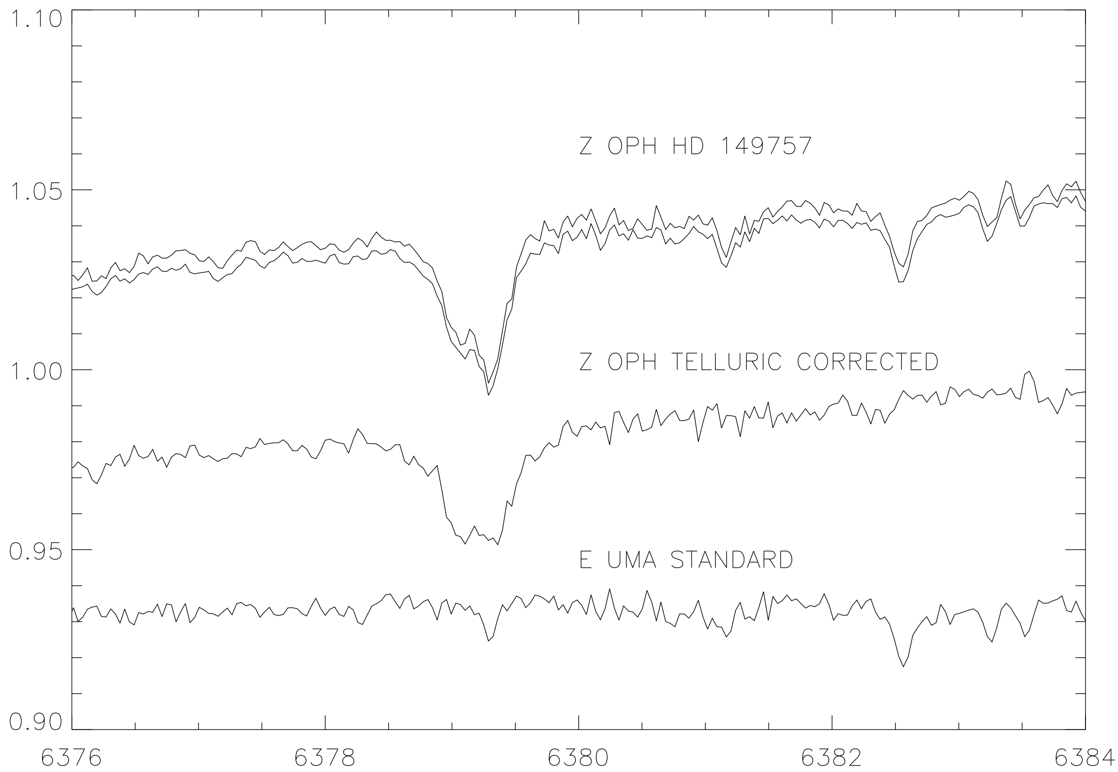
We have also searched for PAH cations and have derived corresponding limits for the presence of the coronene $C_{24}H_{12}$ and the ovalene $C_{32}H_{14}$ cations in space (Ehrenfreund et al. 1995). The abundances of these pericondensed monocations appears to be less than 0.05 % of the cosmic carbon. Ehrenfreund et al. (1995) studied the ionization properties of PAH cations and find that their resistance against UV radiation can produce pathways for selective destruction.

The most remarkable feature of DIBs is their intrinsic broadness (from 1-200 cm^{-1}). If the carrier is a large ion or radical, then the broadening can be due to rotational broadening or lifetime broadening. Measurements of rotational band contours give information on molecular moments of inertia and restrict the identification of carrier molecules. Theoretical contours have been calculated by Cossart-Magos & Leach (1990) for PAHs and Edwards & Leach (1993) for fullerenes, but observational data at high S/N and sufficient resolution are lacking for comparison.

We developed a simple code for calculating contours of P, Q and R branches of electronic transitions of large molecules (such as PAHs and fullerenes) for given moment of inertia of fundamental and excited levels and interstellar rotational temperature. For observed DIBs in series of lines of sight with different temperatures, the variations of the branch separation allow a determination of the moment of inertia.

We recently observed narrow DIBs (5797, 6379 and 6613 Å) with high resolution of R=70.000 and very high S/N (> 500) toward non-turbulent single clouds (at OHP). For lines of sight between 50 - 95 K we find a double peak structure for the 5797 Å DIB with separation of 0.3 Å and a triple peak structure for the 6613 Å DIB with side peaks at -0.26 and +0.34 Å (Foing et al. 1995). These results are consistent with rotational contour calculations of large gas phase molecules (Cossart-Magos & Leach 1990).

Fig. 1 shows the high resolution profile of the narrow DIB at 6379 Å towards ζ Oph. At this S/N an adequate telluric correction is required (observed spectrum of η Uma at the same airmass). The corrected DIB profile at 6379 Å shows two equal peaks separated by 0.25 Å (0.6 cm^{-1}) consistent with a rotational contour of the P and R branch. The observed separation is smaller than calculated by Cossart-Magos & Leach (1990) for molecules like pyrene (separation 2 cm^{-1}) at a kinetic temperature of 70 K, indicating that an asymmetric molecule larger than ovalene (separation 1 cm^{-1}) must be the carrier.



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Search for molecular DIB carriers : laboratory experiments on jet-cooled PAH derivatives

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Polycyclic Aromatic Hydrocarbons (PAHs) derivatives are presently the best candidates proposed as carriers of the 200 unidentified Diffuse Interstellar Bands (DIBs). We have developed a free jet expansion experiment to obtain laboratory fluorescence spectra of cold DIB carrier analogues. PAH cations or radicals whose open shell structures offer visible absorption with a high oscillator strength are expected to be abundant in the ISM. Our first attempt has been made on perylene ($C_{20}H_{12}$), as the fluorescence spectrum from its cation in rare-gas matrices has already been reported. The species formed in the supersonic jet by irradiation with a UV laser beam have time to relax before absorption of a visible photon at tunable wavelength can occur. The absorption* spectrum we got shows a rich set of narrow bands which extends to the blue from 12134.7 cm^{-1} (824.0 nm) and presents a lot of vibronic bands being presently under tentative assignment. The so far uniden! tified species formed from the abs orption of four of the 248 nm photons (KrF laser) by the perylene molecule is fractionated into the fluorescent radical C_2 (Swan emission bands 3-v") by the last visible photon, when it is absorbed. This is thus an interesting mechanism for the formation of C_2 in a precisely defined state.

This experimemt has been built to study the absorption spectroscopy of PAH radicals or cations by using laser induced fluorescence, and it seems to show that the fluorescence quntum yield in $C_{20}H_{12}^{+}$ is probably much smaller than in rare-gas matrices. This quantum yield is an open question for most of the PAH derivatives of interest. From the present results, interesting problems concerning general characteristics of DIBs carriers can be discussed, as the spectra are for the first time directly comparable with the interstellar ones : the species are isolated, cooled and irradiated as in the diffuse medium.

* Indeed action spectrum for excitation of C_2 fluorescence

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Grains of interstellar origin in the heliosphere

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The presence of interstellar dust in the heliosphere was assumed for a long time. Indications come from astronomical observations as well as from meteorite analysis. Until Ulysses, however, dust grains of interstellar origin have never been measured *in situ*. Earlier analysis of the Pioneer 8/9 data in the Earth orbit lead to an upper limit of 3% for the contribution of grains on hyperbolic orbits to the total measured flux. With the highly sensitive impact ionization detectors onboard the Ulysses and Galileo deep space probes it was possible to measure interstellar dust *in situ* for the first time. The interstellar origin of the dust grains is indicated by their speed and impact direction as well as by the almost constant flux independent of the heliocentric latitude of the Ulysses orbit. The measured interstellar dust flux is $1.5 \times 10^{-4} m^{-2} s^{-1}$ with a mean mass of $3 \times 10^{-13} g$ and speeds of approx. 30 km/s. It arrives from an upstream similar to that of the interstellar Helium, which shows that the coupling between interstellar dust and gas is strong. We review the Ulysses and Galileo observations and discuss the dynamics of the interstellar grains.

Laboratory studies of photodissociation and photoionisation processes

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Molecular photodissociation and photoionization is of considerable importance in astrophysics and, more especially, in the interstellar medium in which isolated molecules are mainly subjected to the interstellar radiation in a large spectral range. In the last years, the field of photofragmentation (including both processes, i.e. photofragments of different nature as neutral atoms or molecules, ions and electrons) has undergone tremendous growth. The development of supersonic beams, short laser pulses, VUV lasers, time of flight spectrometers, ..., has provided detailed information on the mechanism of these photofragmentations, involving the excitation step, the unimolecular reaction dynamics and, finally the characterization of the fragment distribution.

This talk focussed on the competing decay pathways for superexcited molecular states below and above the first ionization limit, following photoabsorption. In this energy region, molecular Rydberg states may decay by fluorescence, predissociation or autoionization. In most cases, fluorescence decays are very slow and can be ignored with respect with the two other decay mechanisms. On the other hand, predissociation and autoionization, resulting from interaction of a bound superexcited state with a *nuclear* (i.e., vibrational) continuum state and an *electronic* continuum state, respectively, are generally very fast decay processes. In addition to these competing mechanisms, direct photoabsorption to a dissociation or an ionixation continuum can also occur. Competition between ionization and dissociation will be illustrated by two examples taken from laboratory studies of H_2 and HCl. Finally, the application of a very selective laser technique, the resonant multiphoton ionization (REMPI), to the study of such decay mechanisms will be described on the example of C_2H_2. Photofragmentation of acetylene in the circumstellar clouds is most probably one of the sources for production of carbone and carbonated species in the interstellar medium. Most of the highly excited Rydberg states of this molecule exhibit fast predissociation and, therefore, must play an important role in this fragmentation mechanism. Two-colour REMPI studies were presented and discussed, with the aim of understanding the structure and decay dynamics of these Rydberg states.

High resolution VUV laser measurements of the absorption cross sections of the CO $\mathrm{A}^1\Pi(0 < v' < 17) - \mathrm{X}^1\Sigma^+(v'' = 0)$ transition

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The $\mathrm{A}^1\Pi(0 < v' < 17) - \mathrm{X}^1\Sigma^+(v'' = 0)$ transitions of CO are used to determine the CO column density of diffuse interstellar clouds. These VUV transitions ($117 < \lambda < 154$ nm) were initially observed by Copernicus and IUE and more recently by the HST (1). Comparison of weak high v' bands measured for $^{12}C^{16}O$ and strong low v' bands measured for $^{13}C^{16}O$ or other rare isotopomers allow the determination of isotopic ratios. It is thus extremely important to determine reliable absorption cross sections for a wide range of $v' - 0$ transitions.

A complete set of values was obtained for ($0 \leq v' \leq 12$) in our group by a low resolution optical absorption method (2). These values were in good agreement with those obtained earlier using a lifetime technique for $0 \leq v' \leq 7$(3). Recent low resolution measurements by electron energy loss (4) result in signicantly ($\simeq 30\%$) lower cross sections for $7 \leq v' \leq 12$. Optical absorption measurements for $11 \leq v' \leq 14$ obtained recently at high resolution(5) do not resolve the contradiction.

We have undertaken a systematic set of high resolution measurements using our VUV laser facility which, by 4-wave difference frequency mixing in rare gases, covers the range 117 to 200 nm. We will thus obtain absorption cross sections for $0 \leq v' \leq 17$.

These measurements, which are currently in progess, require a careful treatment of the saturation effects caused by the fact that the laser linewidth (13 mÅ) is markedly larger than the Doppler linewidth (3 mÅ) of the individual rotationally resolved absorption lines (6). These nonlinearities are introduced by the convolution of the instrument function with the exponential Beer-Lambert absorption profile. They are taken into account by a forward modelling technique where a synthetic absorption spectrum of the band convoluted with the instrument profile is least-squares fitted to the experimental spectrum by adjusting integrated-band cross sections spectroscopic data perturbations. The technique is considerably improved by pressure broadening the lines through admixture of about 1000 Torr of Argon at which point the instrumental width is of the same order as the linewidth. This reduces the nonlinearity of the absorption and makes the fit much easier.

Once these effects are correctly taken into account, we obtain reliable results which are directly applicable to the rotationally resolved absorption spectra observed in the interstellar medium. Whatever difference remains with the electron energy loss results will have to be attributed to a failure of the assumed equivalence of electron energy loss and photon absorption cross sections.

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High spatial resolution observations of H_2 vibrational fluorescence in the reflection nebulae NGC2023 and NGC7023

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Using the Canada-France-Hawaii telescope to observe the reflection nebulae NGC2023 and NGC7023, we have obtained 0.8" spatial resolution images of vibrationally excited H_2 in the v=1-0 S(1) line at 2.121 μm and in the v=1-0 S(2) line at 2.033 μm. The images show on both objects narrow filamentary structure (or eddies). These structures show spatial correlations, but also anti-correlations, with the structure of extended red emission (ERE), with implications for the mechanism of ERE.

For NGC7023, spatial variations in the S(1) emission and in the ratio of S(1) to S(2) emission are found in regions lying within a one to a few arcseconds of each other. This is interpreted in terms of small scale structures in the gas in the H_2 emission zone, on a scale of 0.004 pc or less. These data give for the first time the scale-size of structure in the molecular clouds from which stars, such as the central illuminating HD200775 one, have recently formed. Our most recent models of VUV excitation of H_2 IR fluorescence, by light from a nearby star, give a good estimate for the observed peak brightness in the v=1-0 S(1) line.

For NGC2023 earlier observations of H_2 IR fluorescence (Field et al. 1994) around the central star HD37903, have been extended to the North where a new triangular structure has been observed. Its brightness, at this distance of the illuminating star, is not fully understood for the moment. To the South-West a zone of intricated filaments, relevant to PDRs models, appears while a series of Herbig-Haro objects serves as a test for S(1)/S(2) measurements on the filaments.

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Coal analogues for circumstellar and interstellar carbonaceous dust

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There is now a rising evidence that circumstellar and interstellar dust gives rise to a wide diversity of spectral features. This diversity is one of the challenge in the problem of the identification of the nature of the cosmic dust. In the case of the carbonaceous dust, this problem can be approached by taking as model grains of demineralized coal. This choice has been done thanks to the ir absorption spectra of coals that include systematically all the unidendified infrared (UIR) bands and only them /1/. In coal, these bands are due to the functional groups attached to the solid skeleton. The latter is made of basic structural units (BSUs) of graphitic structure (sp2 carbons) embedded in a more amorphous matrix (mainly sp3 carbons). The $\pi - \pi^*$ electronic transition of the BSUs is responsible for a feature near ∼2200Å in the absorbance spectra of coals, that allows to modelise the UV bump in the interstellar extinction curve /2/.

The coal model is all the more interesting because coals form a family of materials, with continuous properties depending on one parameter : the rank (or age). With the age, the coal structure tends to become more and more graphitic (increase of the ratios sp2/sp3 and C/H). The main physical parameter which drives this natural evolution, is the temperature and indeed, such evolution can be reproduced in laboratory through heat-treatment. Roughly, we can define four main stages of evolution of coal: low-rank coals, semi-anthracite, anthracite and semi-graphite. This structural evolution manifests itself in the optical properties of the material. In the UV range, the 2200Å feature is more and more pronounced and shifts toward 2175Å. In the ir range, the bands due to the aliphatic functional groups and to the highly hydrogenated groups diminish. This evolution is striking from semi-anthracite to anthracite, in which the bands at 3.3 μm and at 11.3 μm dominate.

In this paper, we show how the consideration of such a family accounts for the diversity of the astronomical observations in the field of UV extinction as well as ir absorption or emission. Modelisations are based on laboratory measurements of the optical properties (from the UV to the far -ir) of standard coals with different ranks, and do not require supplementary hypotheses.

In the UV/visible extinction field, we show that a mixing of low-rank coals and semi-graphite is able to simulate the mean galactic interstellar extinction curve: both components contribute to the continuum and to the FUV rise, and the semi-graphite is necessary to reproduce the UV bump. Changing the ratio between these components allows similarly to reproduce the curves from the Large Magellanic Cloud and their variations according to the line of sight /3/.

In the infrared range, the consideration of spectra of low-rank coals, semi-anthracite or anthracite allows to reproduce the diversity of the observations, characterised by the variation of the relative intensity between the UIR bands while their positions hardly change with the origin of the spectrum. So, the strong 3.4 μm aliphatic band, observed in absorption in the spectrum of Galactic center ir sources /4/, is very similar to that provided by low-rank coals, i.e. mainly aliphatic (Fig 1). By contrast, higher ranking coals (i.e. more aromatic) are much more representative of the features exhibited by various circumstellar emission spectra. Indeed, the ir spectra of proto-planetary nebulae (PPN) can be adequately simulated with semi-anthracite coal /5/, whereas the "generic spectrum" of UIR bands generally observed in UV excited regions such as planetary is best reproduced with anthracite, a still more evolved coal (Fig. 2).

Thus, from the UV to the ir, the analogy between coal and dust astronomical features suggests that the cosmic grains also belong to a family of materials which, as coals, can change in time and according to the environment.

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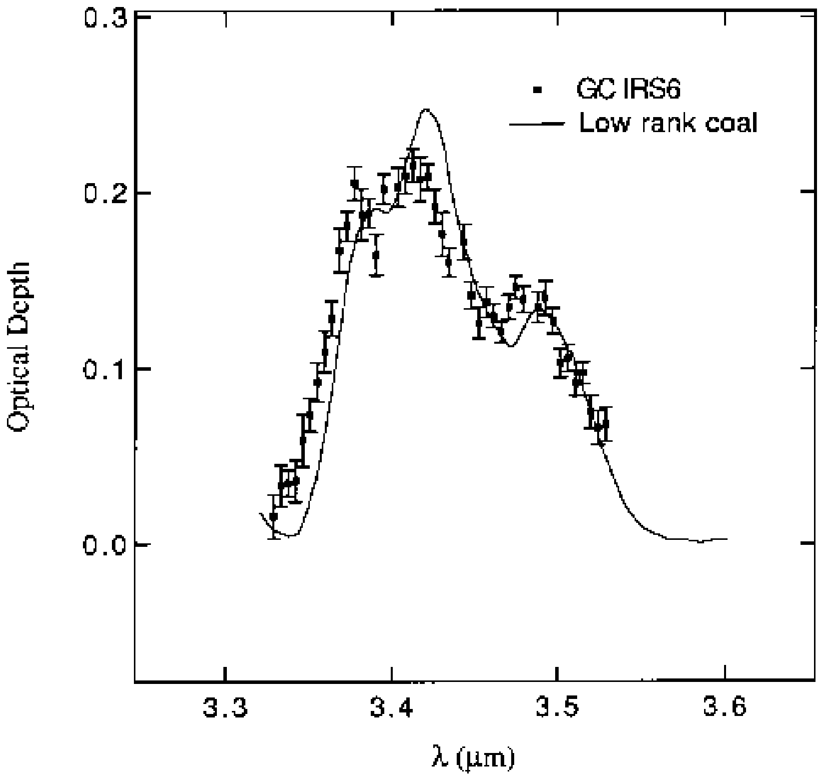

Figure 1. Comparison of the optical depth spectrum of the Galactic center source IRS 6E /4/ to the near-ir absorbance spectrum of a low-rank coal.

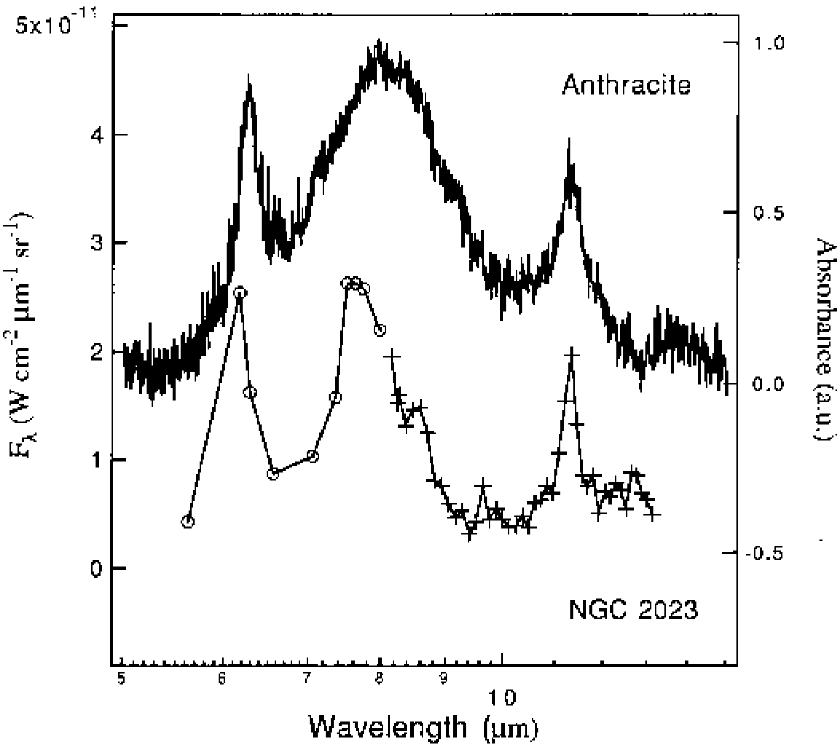

Figure 2. The mid-infrared absorbance spectrum of anthracite coal compared with the corresponding part of the emission spectrum of the reflection nebula NGC2023, adapted from Roche et al, MNRAS 269, 649 (1994).

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Chemistry in shocks : the gas-grain interface

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We shall present models of C-type shocks that include the dynamical and chemical effects of PAH molecules (1) and the chemical and thermal effects of adsorption to and desorption from grains (2). We find that the sputtering associated with the relative motion of the ions and the neutrals within the shock can completely remove the grain mantles for shock velocities as low as 20 km/s.

In particular, the column densities of molecules such as NH_3 can be greatly enhanced by sputtering, assuming that saturated molecules are produced in the mantle. C-shocks are able to reproduce the metastable levels of ammonia up to (J,K) = (14,14) that have been observed in absorption towards SgrB2, a giant molecular cloud close to the galactic centre (3).

At higher velocities, C-shocks propagating in molecular clouds can sputter the refractory materials which compose the cores of interstellar grains (4). Current estimates of the sputtering yields suggest that the cores can be at least partially destroyed at shock velocities of only 50 km/s. In view of their importance, the yields are being recalculated for the sputtering of silicates and graphite by He impact (5). At high shock velocities, the electrons become sufficiently hot to electronically excite the H_2 molecules, giving rise to either dissociation of the molecule or to UV fluorescence, which ionizes the gas. As a consequence, the shock width decreases when the shock speed rises. The rate of momentum transfer between the ionized and neutral fluids regulates the shock profile.

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Ice Cocktails in Molecular Cloud Cores

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An important goal in star formation studies is to understand the structure and composition of protostellar envelopes, in order to determine the properties of the embedded young stars and their disks.

The main motivation for this work has been the need to constrain the parameters going into the current models of core collapse and star formation. One way of probing the physical conditions along the envelope is by comparing the observed column densities of silicates and ices with the results of protostellar models. Moreover, the profiles of those features may provide information on the composition, structure and thermal history of the grains (for a review see Whittet & Duley 1991).

Solid CO in grain mantles is identified by an absorption feature at $4.67\mu m$, corresponding to the fundamental stretching mode of the CO molecule. As shown by laboratory studies (Sandford et al. 1988, Schmitt et al. 1989), the peak position and width of the solid CO band depend on the chemical composition of the icy matrix in which CO is embedded, and on the extent of thermal processing of the ices. The observed features toward dark clouds generally show two components: a narrow dominant one at $\sim 4.674\mu m$, and a broader weaker feature at $\sim 4.681\mu m$ appearing as a long wavelength wing. The dominant component is due to CO in a nonpolar environment (CO, CO_2, O_2, N_2), and the broader one can be explained by CO trapped in polar mixtures (H_2O-dominated).

These two types of ices present in the mantles may point to different stages in the grain mantle evolution, which lead to an "onion" skin structure of the ice mantle (Tielens et al. 1991). Initially, at low densities ($n_H < 10^4 cm^{-3}$) and in atomic hydrogen rich conditions, the H_2O-rich ices form on the grain. As the grain enters a dense core, or as the core contracts and the density increases ($n_H > 10^4 cm^{-3}$), the conditions become inert or oxidizing, most of the hydrogen will be in the molecular form and the ices now formed will be dominated by nonpolar molecules.

In this work, 4.5 - 4.9 μm spectra were taken with CGS4 at the UKIRT, toward embedded Young Stellar Objects in the Taurus, Perseus and L1641 molecular clouds. The solid CO band was detected in 6 of the 13 observed sources: B5 IRS1, L1489, L1524, Re50N IRS1, SVS12, and TMC1A. An attempt has been made to determine the likely composition of the CO ices by comparison of the observed features with laboratory data from Sandford et al.(1988), Schmitt et al.(1989), and Tielens et al.(1991). The result of χ^2- minimization is shown in fig.1 for two of the sources.

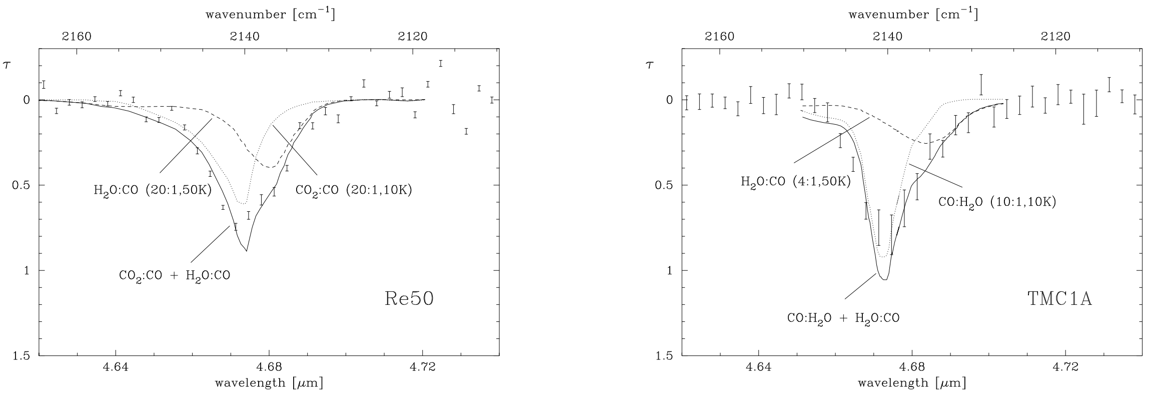

Fig.1 Spectra of Re50N IRS1 and TMC1A in optical depth units, and best laboratory data fits (solid lines). The dotted and dashed lines correspond to the nonpolar and polar components of the ice mixtures, respectively.

A forming star heats up its surroundings, creating a temperature gradient along the protostellar envelope. That will cause the composition of the grain mantles in the envelope to vary with the distance to the centre. Closest to the star the temperature is too high for any grains to survive. For radii where the temperature drops below $\sim$ 2300 K, bare grains can exist but their icy mantles will have evaporated. Farther out, in regions of T $\leq$ 100K, the grains will have H_2O-rich mantles, with increasing trapped CO content as the temperature decreases. In the coolest outer parts of the envelope, where T $<$ 20 K, pure CO and other very volatile nonpolar ices can also survive in the grain mantles.

The Adams, Lada & Shu(1987, hereafter ALS) model for a low mass protostar, produces a density and a temperature profile along the envelope. Integrating over the range of temperatures where CO can exist in the grain mantles, the total CO column density was estimated from the model, assuming 75% by mass of H_2 in the gas and $N(CO)/N(H_2) = 8 \times 10^{-5}$ (Frerking et al. 1982, van Dishoeck et al. 1993). Figure 2 plots the total CO column density estimated from the model, $N(CO)_{ALS}$, against the solid CO column density derived from the spectra, $N(CO)_s$, for some YSOs in this study and from the literature. It can be seen that for some sources there is more *observed solid* CO than the *total* amount of CO *predicted* to be available. The reasons for this discrepancy might involve *a)* the CO to H_2 ratio which might be higher in star forming cores due perhaps to a different chemistry, *b)* the density profile along the envelope which might be shallower than that assumed by ALS, and *c)* the size of the core assumed in the model which might also be larger. It is, however, acknowledged that it is difficult to assess whether all the material in the line of sight belongs to the collapsing core or if a part of it belongs to the quiescent molecular cloud.

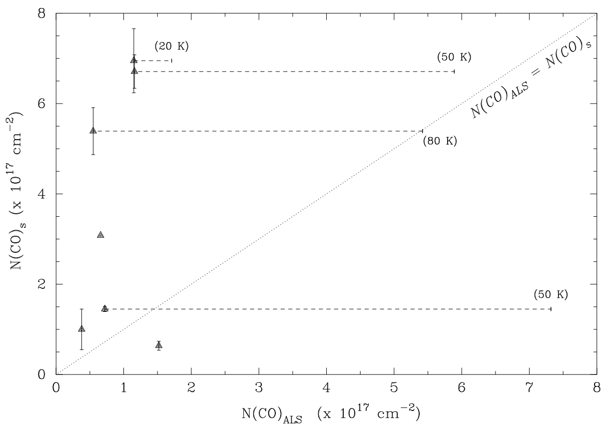

Fig.2 Observed solid-CO column density ($N(CO)_s$) *vs.* predicted total (gas+dust) CO column density using the ALS model for a protostar. The triangles correspond to integrating the model for temperatures below 17K. The integration was also allowed to proceed up to the temperature indicated by the polar component of the mixture, for the sources for which laboratory fits were possible. The result of that integration is given by the dashed lines.

Finally, the possibility of using the ice mantles as probes of early activity in the embedded stage of the life of a star is being explored. The processes that may cause warm up of the grains around a forming star are being analysed. This analysis may lead to a new way of detecting such activity from the profile of the solid CO band.

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Molecular environments in astrophysics

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A remarkable amount of chemical activity takes place in interstellar clouds, circumstellar envelopes, comets, and other astronomical phenomena, despite the low temperatures (often less than 100 K), the low densities ($10^2 - 10^6$ cm^{-3}), and the exposure to harsh starlight and cosmic rays. This review will concentrate on recent developments in the investigation of interstellar chemistry, with particular emphasis on the photon-dominated regions (PDRs) where ultraviolet starlight plays an important role in the chemistry and molecular excitation.

Recent work on observations and modeling of PDRs will be reviewed. In PDRs such as the reflection nebula IC 63, the abundances of many molecules can be understood. Persistent discrepancies may, in some cases, be related to the difficulty of treating the transport of radiation through a turbulent medium. Some future prospects for characterizing the turbulence and small-scale structure will be discussed. Diffuse and translucent molecular clouds are thought to be PDRs throughout: even in these ostensibly simple systems, some chemical mysteries remain. Recent attempts to explain the ubiquity and high abundance of the reactive ion CH^+ center on a high-temperature chemistry related to the turbulent component.

Perhaps the most extreme form of PDR is the kind that must exist in the high-pressure region of a galaxy with a central starburst, in which gas concentrations of the order of 10^9 solar masses or more are being transformed into stars at a high rate. Interesting radiative environments exist in these regions, in some cases supporting the existence of luminous H_2O masers very close to an active nucleus (non-thermal radiation source).

The response of H_2 to X-rays

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ABSTRACT: The rates of population of the rovibrational levels of H_2 by the impact of energetic photoelectrons produced by the absorption of X-rays are calculated. Population occurs by excitation of electronically excited states of H_2 followed by cascading and by direct impact excitation of the lowest vibrational level. The resulting infrared spectra are obtained. The emission from high vibrational levels is similar to that from ultraviolet pumping. Emission from the v=1 and 2 vibrational levels in a gas of low fractional ionization is dominated by direct electron impact excitation. The intensity ratio of the $S(1)(2,1)$ and $S(1)(1,0)$ lines is 0.06 in a gas of low fractional ionization and 0.54 in a gas of high fractional ionization.

3-D spectroscopy of planetary nebulae in the infrared

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The comprehensive study of extended and complex sources like Planetary Nebulae (PN) which contain, dust ring, ionised region, molecular envelope, supposes the use of 3-D techniques. Ideally, to separate and qualify all these components, the appropriate spatial and spectral resolution and the largest possible spectral coverage are needed. None of the current optical instruments could have these properties altogether, particularly in the infrared. With the advent of infrared bidimensional array detectors, the throughput advantage of a Fourier Transform Spectrometer can be exploited to create a 3-D spectrometer which has many advantages. A NICMOS 3 array has been coupled to a FTS at the CFH telescope. With this combination, spectro-imaging in any bandpass between 1 and 2.5 μm is made possible within a circular field of 24 arcsec, with a plate scale of 0.33 arcsec/pixel, at seeing-limited spatial resolution. The spectral resolution is adaptable from very low up to 10 km/s over the full field. A description of this technique is presented in a first part.

Three typical PNs, NGC 2688 and NGC 7027 in the early phases, to a more evolved object, BD+30°3639, have been studied with this instrumentation. They represent three different stages of evolution from AGB to PNe which can be clearly identified. The observations have been concentrated on the K' band, which is dominated by several H_2 lines. Six lines of the 1–0 and 2–1 bands, with among them the strongest one, 1–0 S(1) at 2.12 μm, give access to the morphology, the kinematics and the exitation conditions of the molecular envelope. Comparisons with molecular images from millimetric data become possible. In the same band, Bγ (2.16 μm), HeI (2.06 and 2.11 μm) and HeII lines (2.19 μm) are also accessible, to study in the same way the ionized region when present. In addition, pure images in the continuum, with no contamination by the line content, can be derived to study the morphology of the scattered light. All these results illustrate the richness of this spectro-imagery in the infrared.

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Molecular abundances at the onset of dark-cloud chemistry

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With the Plateau de Bure Interferometer we have observed the millimeter-wave absorption lines of a few simple molecules in Galactic interstellar clouds, seen in front of seven distant quasars. Seventeen individual clouds have been are observed; although we have no direct measurement of the molecular hydrogen column densities, we have indications that they sample the transition range between diffuse clouds and dark clouds. The detected species are ^{12}CO, ^{13}CO, HCO^+, $H^{13}CO^+$, HCN, HNC, CN, C_2H, C_3H_2 (ortho and para species), CS, SiO, and SO.

Due to the very low excitation levels (most of these molecules are not seen in emission), we are able to derive accurate column densities. The CO turn on is clearly seen as in optical absorption studies; we show that some molecules follow the same behaviour as CO, while others, just like HCO^+, are still abundant at lower column densities.

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Electronic Supplement – Conference Posters

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Brief abstracts and extended summaries for most of the posters presented at the First Franco-British Meeting on the Physics and Chemistry of the Interstellar Medium are available in a supplement to this Newsletter. This is published in electronic form and can be recovered as a postscript file either by:

ftp: ccp7.st-and.ac.uk:/ccp7/News_22/Supp22.ps

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R.Bocquet, J.M.Colmont, J.Cosleou, J.Demaison, G.Wlodarczak
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