#### Molecules in the interstellar medium

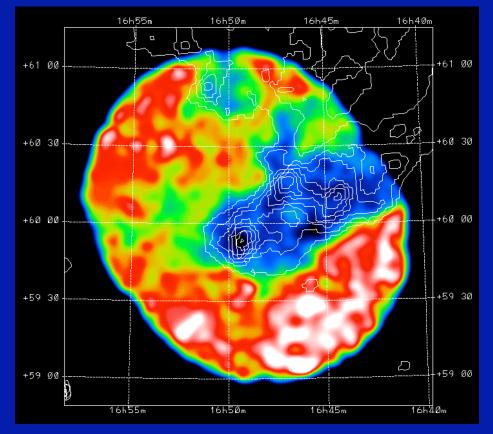
The ISM: composition, mass, energy flow, and synthesis of the interstellar molecules

## Composition of the ISM



- The interstellar medium (ISM) consists of gas and dust existing over a wide range of physical conditions
- About 1/2 of the ISM mass in our Galaxy is molecular in form
- The ISM is powered by energy emitted by stars (SN, giant stars, novae, etc.)
- The 5 ISM components: "coronal" gas, warm intercloud medium (WIM), HII regions, neutral hydrogen (HI) clouds, and complexes of giant molecular clouds (GMCs)

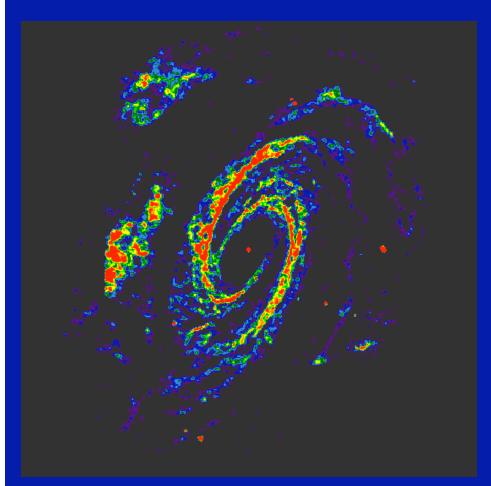
#### Coronal gas and the WIM



From D. Burrows, PSU

- Coronal gas is observed as far-UV absorption lines of highly ionized atoms and in the form of a soft X-ray background
- It is hot (log T> 6), rarified (log n < -1.5), and has a filling factor as large as 0.5
- It is a product of hot gases ejected in stellar explosions and winds
- The WIM occupies most of the rest of the Galaxy. It is seen as broad emission features in HI spectra of extragalactic sources
- The WIM has: log T<4 and -1.0< log n < 0</li>

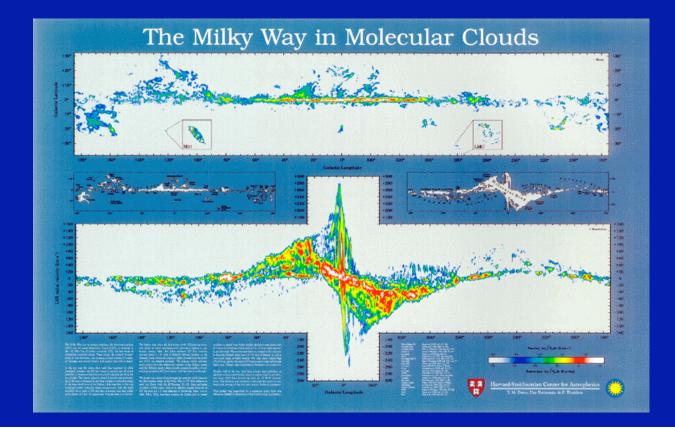
#### Neutral hydrogen (HI) clouds



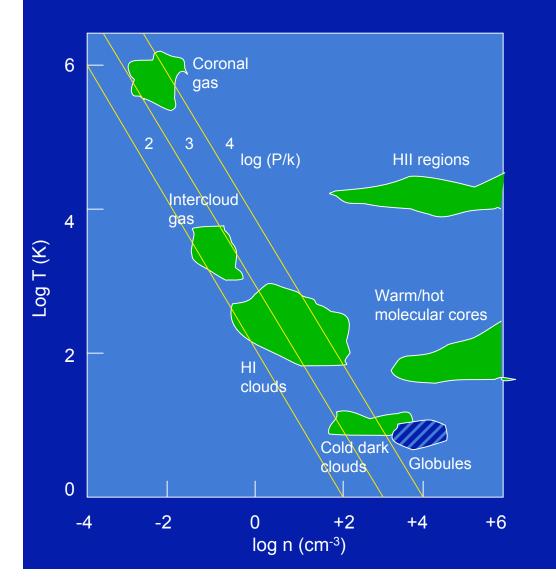
- Roughly another half of the mass of the ISM is in HI clouds
- HI is observed at 21 cm (1420 MHz) as the result of a low-probability transition (electron spin flip) in the hyperfine structure of the ground energy level of H
- HI clouds have log T<2. Because of their abundance, they have been used as excellent tracers of spiral structure
- HII regions are small, roughly spherical clouds of hot (log T~4) ionized H, centered on hot stars (sources of ionizing UV radiation)

#### Molecular clouds

- GMCs are complex (sizes 20-200 pc), massive (10<sup>3</sup>-10<sup>7</sup>M<sub>sun</sub>), cool (T<10K) regions, which are sites of chemical and dynamical activity leading to star formation
- Their mean density estimates vary from 10<sup>2</sup> to 10<sup>3</sup> cm<sup>-3</sup>
- GMC structure is best traced by mapping the emission of collision excited <sup>12</sup>CO molecule

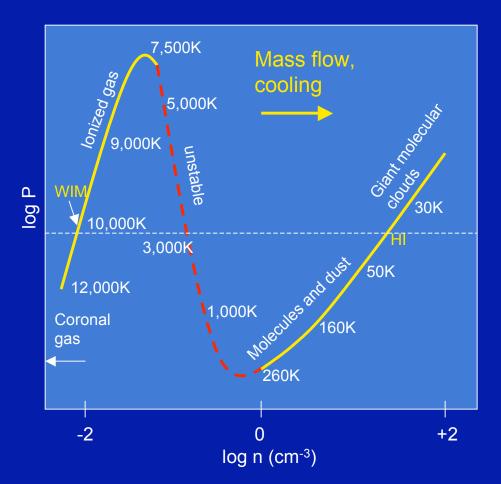


## Morphology of the ISM



- Temperatures and densities of the main components of the ISM keep them in an approximate pressure equilibrium
- GMCs and HI clouds are comparable in total mass and are more massive than the intercloud gas (WIM), which contains much more mass than the coronal gas
- Most of the galactic volume is taken by the coronal gas and the WIM, followed by HI clouds and the GMCs, which are the most compact ISM structures

## Dynamics of the ISM

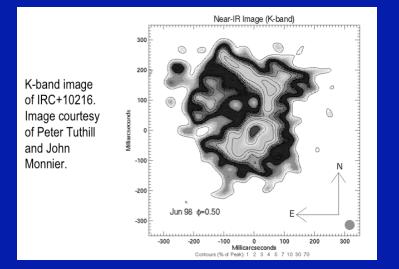


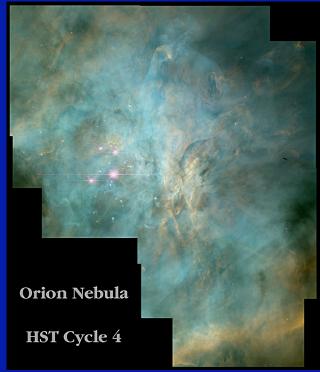
- Energy and mass relationships in the ISM can be schematically depicted as a pressure-density diagram of its main components
- They are located on the line of dynamical equilibrium (T,P vs. n)
- Coronal and HII phases (not shown) are not in equilibrium (both fed by stellar activity)
- Global pressure balance exists between the WIM (fed by coronal gas) and HI phases of the ISM
- In the region of instability, neutral, atomic gas reradiates energy under compression --> spontaneous collapse
- Stability of GMCs is maintained by gravity (no consequence for the global ISM equilibrium)

## The basic interstellar chemistry

Production of molecules in the interstellar space

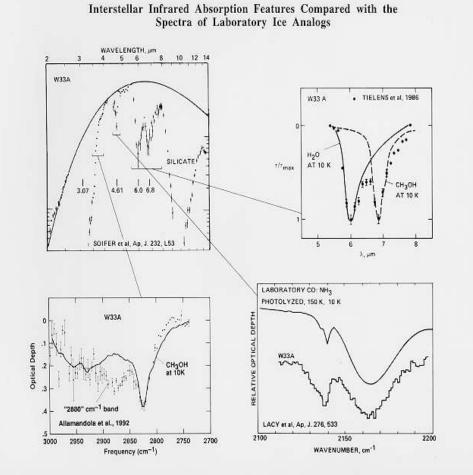
## Fertilization of the ISM





- Interstellar chemistry begins with the formation of dust grains in the outflows from giant stars
- In the process, all Si and Fe, 50% of C and 20% of O get locked up in dense dust grain cores and become chemically inert
- Over 120 molecules have been identified in the ISM. It is clear that the interstellar chemistry is carbon-dominated (e.g. cyanopolyynes, PAH's)
- Molecules form in a variety of environments (diffuse ISM, circumstellar shells, GMCs)

#### What do we get out of spectral lines?

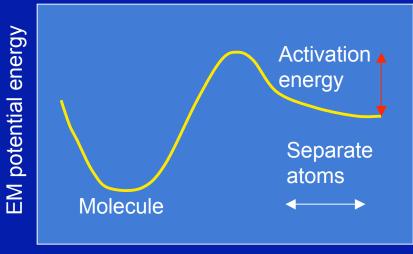


- Most of the interstellar molecules are detectable at mm wavelengths through emission/absorption generated by their rotational states
- Solid state molecules (ices) are detectable in IR (vibrational states)
- From radiative transfer:

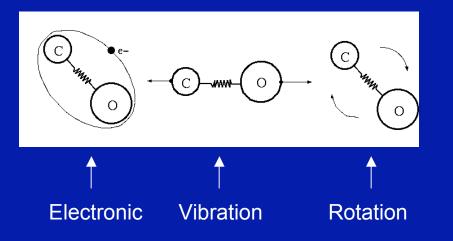
$$\begin{split} I_{\nu} &= B_{\nu} T_{ul} (1 - e^{-\tau_{\nu}}); \quad \tau_{\nu} = n_{l} \alpha_{\nu} \\ \Delta T_{B} &= (T_{ul} - T_{bg}) (1 - e^{-\tau_{\nu}}); \quad h\nu << kT \\ \Delta T_{B} &= T_{ul} - T_{bg}; \quad \tau_{\nu} >> 1 \\ \Delta T_{B} &= n_{l} \alpha_{\nu} T_{ul}; \quad \tau_{\nu} << 1 \end{split}$$

- Abundance is derived by integrating *T<sub>B</sub>* over velocities
- Kinetic temperature, T<sub>k</sub> can be computed, if environment is collision dominated: T<sub>k</sub>~T<sub>ul</sub>. Usually obtained from brightness of <sup>12</sup>CO line
- Densities are obtained from unsaturated lines with  $\tau_v >> 1$

## Molecule formation - I



Distance between atoms

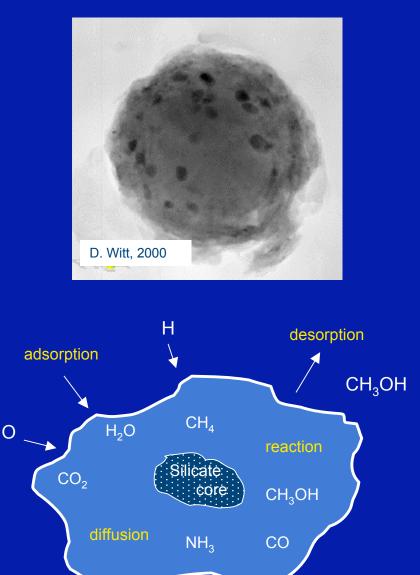


- Chemical bonding involves sharing electrons, therefore it uses electromagnetic, not nuclear forces
- Stable molecule has to have lower EM potential energy than the sum of separate atoms that make it up
- Electrostatic repulsion of electrons form a barrier called the activation energy
- Excitation and energy release by a molecule occurs through one of the three mechanisms: electronic, vibration, and rotation with rotation being important in the gas phase and vibration dominating in the solid state environment (ices on top of dust grains)

## Molecule formation - II

- Gas-phase, ion-molecule: cosmic rays ionize H<sub>2</sub>, make H<sub>2</sub><sup>+</sup>, H<sup>+</sup> (also He<sup>+</sup>), which react with H<sub>2</sub> and CO (most abundant) and create simple neutral molecules and metal ions through successive reactions [A<sup>+</sup>+B-->C<sup>+</sup>+D]. Important in both diffuse and dense clouds
- Shock-induced: gas heating caused by shock wave overcomes activation barriers, enables neutral-neutral reactions [A+B-->C+D] that are impossible in cold clouds, may cause grain disruption. Important in dense, hot star-forming regions
- Circumstellar: "freeze-out" chemistry in circumstellar envelopes, gas-phase molecules stick to grains, which develop icy mantles. Reactions proceed on grain surfaces (hydrogenation of O, C, N, formation of H<sub>2</sub> most common, because of H mobility)
- Dust grain surfaces: shield molecules from UV radiation field, produce H<sub>2</sub> through catalysis: H+H+grain-->H<sub>2</sub>+grain (reaction is exothermic, energy is used to detach H<sub>2</sub> from surface). H<sub>2</sub> drives much of gas-phase chemistry

#### Processes on dust grains - I



Adapted from: Ehrenfreund et al, 2005

- Adsorption or sticking efficiency is thought to be high for dust grains. Sticking occurs, when an approaching particle loses energy to the surface's lattice
- Scanning or mobility of particles on surfaces is necessary to produce chemical reactions (quantum tunneling,  $\tau_q = 4h/\Delta E$ , or thermal hopping,  $\tau_h = v^{-1} exp(T_B/T)$ )
- Desorption: micro-continuous---> exothermic reaction liberates molecule (possibly also neighboring molecules) from surface; macro-continuous---> explosive liberation of molecules by mantle destruction by energetic photons or cosmic rays; violent desorption --> collective destruction of grains by shock waves

#### Processes on dust grains - II

- Atoms of H scan the grain's surface fast compared to other atoms, because of their much higher mobility
- Most common reactions: hydrogenation of C, N, O, and H<sub>2</sub> molecule formation in clouds containing enough H:

 $C \Rightarrow CH_4$ : methane  $N \Rightarrow NH_3$ : ammonia  $O \Rightarrow H_2O$ : water

• In high H-abundance clouds, these molecules and CO accreted from gas phase form grain mantles. Low H-abundance limits hydrogenation and allows formation of more complex molecules:

$$O + H \Rightarrow OH \xrightarrow{+C} COH \xrightarrow{+3H} CH_3OH : \text{ methanol}$$

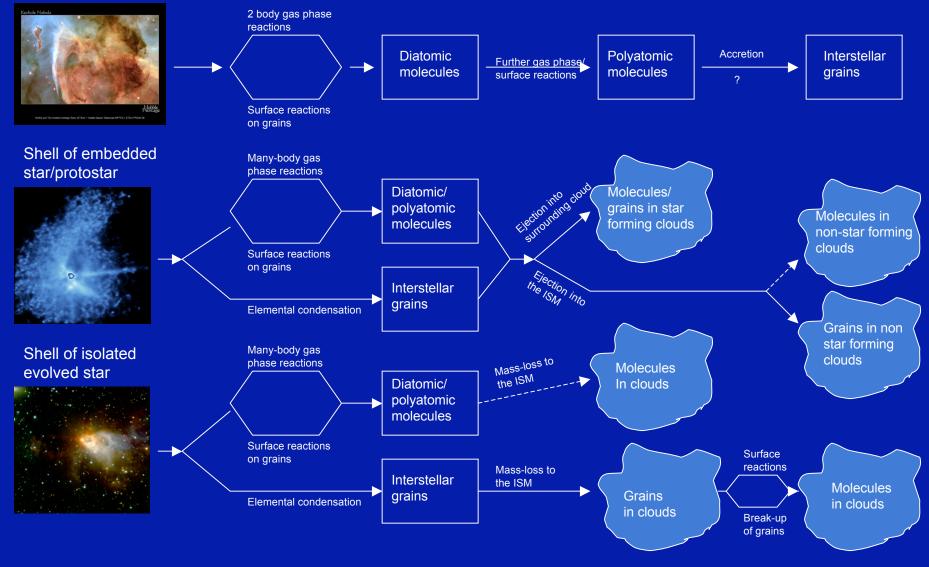
$$CH + H \Rightarrow CH_2 \xrightarrow{+O} H_2CO : \text{ formaldehyde}$$

$$C + H \Rightarrow CH \xrightarrow{+COH + 4H} CH_3CH_3OH : \text{ ethanol}$$

- In absence of atomic H, mantles are formed out of atoms of C, N, O which will react to form O<sub>2</sub>, CO, and possibly NO
- Generally, surface reactions produce simple molecules, while UV irradiation leads to formation of complex molecules

## Molecule formation pathways

Interstellar cloud

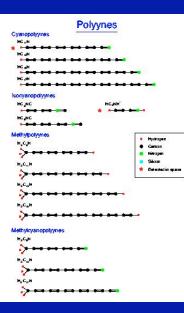


Adapted from: Turner & Ziurys 1988

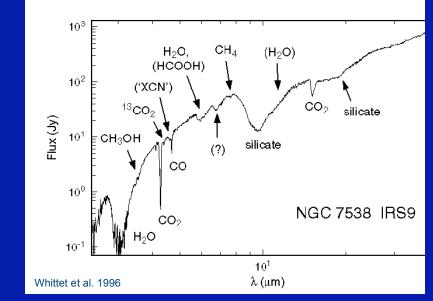
# Examples of molecules in the ISM

#### **OUT OF THIS WORLD** A wealth of molecules is found in interstellar clouds

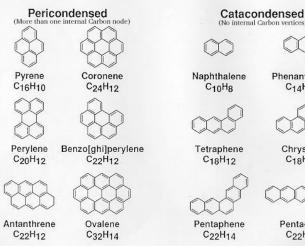
ALF ALCL CH CH CN CO CO CO CO CO CP CSI HCL KCL	ms NO NS NaCl OH PN SO SO <sup>+</sup> SiN SiO SIS CS HF SH FeO	3 atoms C <sub>3</sub> MgCN C <sub>2</sub> 0 N <sub>2</sub> H' C <sub>2</sub> 0 N <sub>2</sub> H' C <sub>2</sub> 5 N <sub>2</sub> O CH <sub>2</sub> N <sub>3</sub> CN HCN OCS HCO SO <sub>2</sub> HCO <sup>+</sup> C-SiC HCS <sup>+</sup> CO <sub>2</sub> HCC <sup>+</sup> NH <sup>2</sup> H <sub>2</sub> O H <sub>3</sub> <sup>-</sup> SiCN HNC AINC	4	l-C <sub>3</sub> H C <sub>3</sub> N C <sub>3</sub> O C <sub>3</sub> S C <sub>2</sub> H <sub>2</sub> HCCN	ms HN( H <sub>2</sub> C H <sub>2</sub> C H <sub>2</sub> C NH <sub>3</sub> O NH <sub>3</sub> SiC <sub>3</sub>	C4 0 C4 N L-C S c-C + CH	H 3H2 3H2 2H1 2CN	H2NCN
	$\begin{array}{ccc} & 6 \ atoms \\ C_5 H & CH_3 SH \\ I_{c} H_2 C_4 & HC_3 NH^* \\ C_7 H_4 & HC_2 CH0 \\ CH_3 CN & NH_2 CH0 \\ CH_3 NC & C_5 N \\ CH_3 OH \end{array}$		$\begin{array}{c} \textbf{7 atoms} \\ C_6H \\ CH_2CHCN \\ CH_3C_2H \\ HC_5N \\ HC0CH_3 \\ NH_2CH_3 \\ c-C_5H_4O \end{array}$		8 atoms CH <sub>3</sub> C <sub>3</sub> N HCOOCH <sub>3</sub> CH <sub>3</sub> COOH C <sub>7</sub> H CH <sub>2</sub> OHCH0		9 atoms CH <sub>3</sub> C <sub>4</sub> H CH <sub>3</sub> CH <sub>2</sub> CN (CH <sub>3</sub> ] <sub>2</sub> O CH <sub>3</sub> CH <sub>2</sub> OH HC <sub>2</sub> N C <sub>8</sub> H	
NOTE: Evidence suggests that much larger molecules such as polycyclic aromatic hydrocarbons and fullerenes are also present. SOURCE: National Radio Astronomy Observatory		0	10 atoms CH <sub>2</sub> CH0H 10 atoms CH <sub>3</sub> C <sub>5</sub> N ICH <sub>3</sub> I <sub>2</sub> CO NH <sub>2</sub> CH <sub>2</sub> COOH		11 aton HC <sub>9</sub> N	ns	<b>13 atoms</b> HC <sub>11</sub> N	

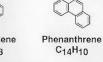


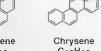




#### **PAH Structures**











## The Grand Scheme



#### Homework #3,4 Deadline: Apr 6

- Write a paper on the following subject: "Organic material from space on Earth: delivery, composition, and relevance to the origins of life". Technical specifications are the same as for paper #1
- Download a set of radial velocity data from the course webpage and analyze it to estimate the five Keplerian orbital parameters of a planet around a star for which these measurements have been made. Given the model orbit, estimate a minimum mass of the planet and its distance from the star. Use information on orbit determination included in the course lecture on the radial velocity method. As before, the more accurate your answers, the better grade you get!