Spectral Line Topics

Taking the Measure of Interstellar Clouds

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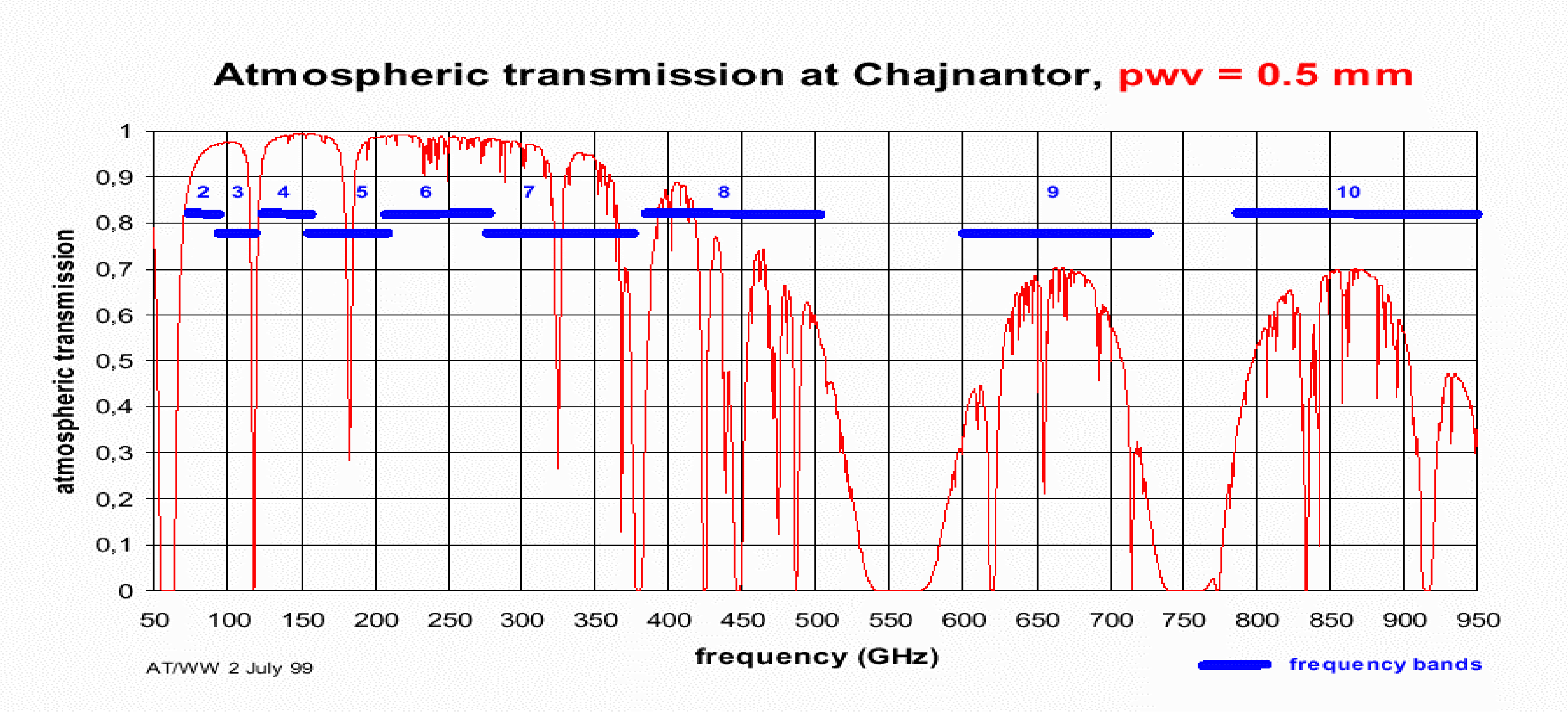
Measurement Goals

- Assess or quantify the physics of interstellar matter Ref: *Evans, Neal, II 1999, ARA&A, 37, 311*
  - Temperature
    - Where are the energy sources and how is that energy transferred to matter?
    - What is the character of the energy sources?
  - Density
    - What is the role of gravity within the cloud and how does that relate to the energy sources?
    - What is the probable course of evolution of the cloud?

Measurement, cont.

- Evolutionary state of matter itself
  - What are the relative atomic and molecular abundances within the cloud?
  - How do those abundances change with location?
  - How do isotopic abundances vary
- Use observable quantities to limit more intangible quantities—better astronomy through chemistry…
  - Electron abundances
  - Ionization rates

Atmospheric Frequency Access



N.B. Band 1 31.3-45 GHz not shown; this plot not very relevant for Green Bank…

Imposition of the Instrument

- The subject of this school—how the instrument interacts with the measurement process; and how an understanding of that interaction brings us closer to an absolute measurement.
- For densities and temperatures, we will generally measure *line ratios,* quantities very sensitive to errors in calibration!
- The good observer is a pessimist, difficult to convince of the truth of his measurement!
- Particularly important effects
  - **Resolution**—always we average over space
    - Along and orthogonally to the line of sight
  - **Missing flux**, the bane of interferometry (Stanimirovic)
    - Interferometric line ratios almost always suspect!
  - **Excess flux** and stray radiation (Lockman)
  - **Calibration** (O'Neil, Jewell)
    - Brightness temperature generally the quantity of interest
    - Varies with instrumental setup
    - Frequency—What *really* is the Tcal value?? Measure it!
    - Instrument—pointing, sag, polarization squint, many other factors

Remedies…or perhaps only Salves

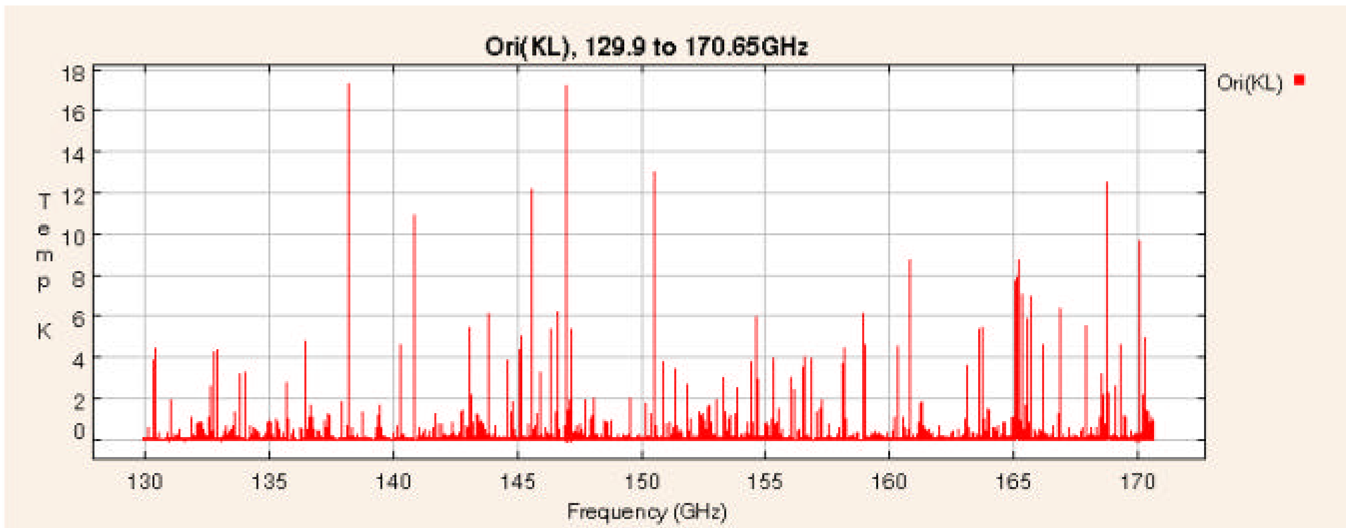
- One instrument combining interferometry and total power
  - Sporadically employed with BIMA
  - A planned feature of **ALMA**
  - Even then, some poorly sampled spatial dimensions
    - Arrays of different antenna sizes
      - CARMA
      - The ALMA Atacama Compact Array
    - Cross-calibration of array and total power telescope hard
- Or a mammoth monolithic telescope…

The Cast

- 128 known interstellar molecules, several atomic lines, notably HI, CI, CII and NII.
- In general, heavy molecules have low frequency lines, light ones well spaced and at higher frequency
- The ideal probe will have qualities which aid measurement
  - High abundance (we want to see it)
  - Lines of different energy levels lying close in frequency
  - Chemically robust (e.g. not only found in alien life forms—glycine?)
  - Several useful transition clusters low within the telescope frequency window (good efficiency) and away from atmospheric absorption.
  - Isotopomers with isotopes of relatively similar abundance (however, we will find interesting aspects of deuterium chemistry…), spin states, hyperfine structure
  - Appropriate 'Characteristic density' – radiative de-excitation equals collisional excitation

H_2	C_3	c-C_3H	C_5	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N	HC_9N			$HC_{11}N$
AlF	C_2H	*l*-C_3H	C_4H	*l*-H_2C_4	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$		C_6H_6 ?		
AlCl	HCN	C_3N	C_4Si	C_2H_4§	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	$HOCH_2CH_2OH$				
C_2	C_2O	C_3O	*l*-C_3H_2	CH_3CN	HC_5N	C_7H	CH_3CH_2OH					
CH	C_2S	C_3S	*c*-C_3H_2	CH_3NC	$HCOCH_3$	H_2C_6	HC_7N					
CH^+	CH_2	C_2H_2	CH_2CN	CH_3OH	NH_2CH_3	CH_2OHCHO	C_8H					
CN	HCO	CH_2D^+?	CH_4	CH_3SH	*c*-C_2H_4O							
CO	HCO^+	HCCN	HC_3N	HC_3NH^+	CH_2CHOH							
CO^+	HCS^+	$HCNH^+$	HC_2NC	HC_2CHO								
CP	HOC^+	HNCO	HCOOH	NH_2CHO								
CSi	H_2O	HNCS	H_2CNH	C_5N								
HCl	H_2S	$HOCO^+$	H_2C_2O									
KCl	HNC	H_2CO	HNCCC									
NH	HNO	H_2CN	H_2NCN									
NO	MgCN	H_2CS	H_2COH^+									
NS	MgNC	H_3O^+	SiH_4									
NaCl	N_2H^+	NH_3										
OH	N_2O	SiC_3										
PN	NaCN	CH_3*										
SO	OCS											
SO^+	SO_2											
SiN	c-SiC_2											
SiO	CO_2*											
SiS	NH_2											
HF	H_3^+											
FeO?	H_2D^+											
SH	AlNC											
CS	SiCN											

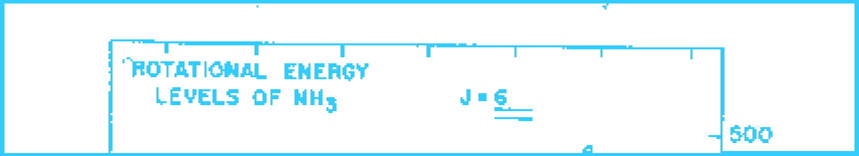
The Interstellar Molecular Zoo
By Number of Atoms



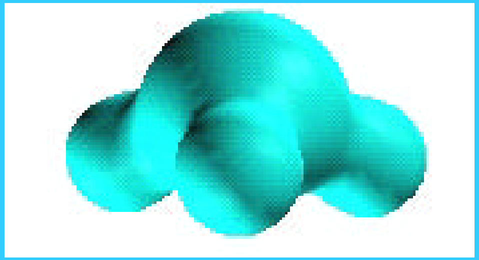
‘Symmetric Tops’

- Their structure is top-like—symmetric—hence simplified spectrum
- Often, lines of differing energy lie within one receiver band
  - Simplifies calibration (e.g. pointing, efficiency) if multiple lines observed at once
  - Time-efficient
- Examples
  - NH_3 Inversion transitions at ?~1cm
    - Problems—light, so widely spaced in energy, good temperature, poor density indicator
    - Advantages—chemically robust, N atom so possesses hyperfine components
    - Many deuteration possibilities; NH_2D, ND_2H, ND_3 seen! Also ^{15}N.
      - **BUT** different symmetries, mixed rotation and inversion transitions
  - CH_3CN Several ‘K’ ladders close in frequency
    - Disadvantages—
      - chemistry favors high temperature formation, so used to monitor hot cores of clouds
      - uncommon
  - CH_3C_2H Closely spaced ‘K’ ladders
    - Disadvantages—
      - chemistry favors high temperature destruction, less often used
      - uncommon

Ammonia, an asymmetric top molecule, has a number of inversion lines lying close together in frequency near 1.3cm. The two lowest observable energy transitions lie at energies of 23 K and 64 K above ground.

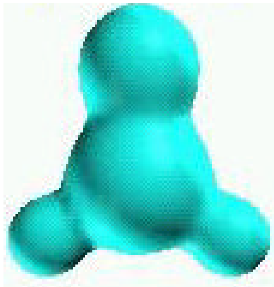


Even with antiquated correlators, these two and maybe more transitions may be observed simultaneously.



Others

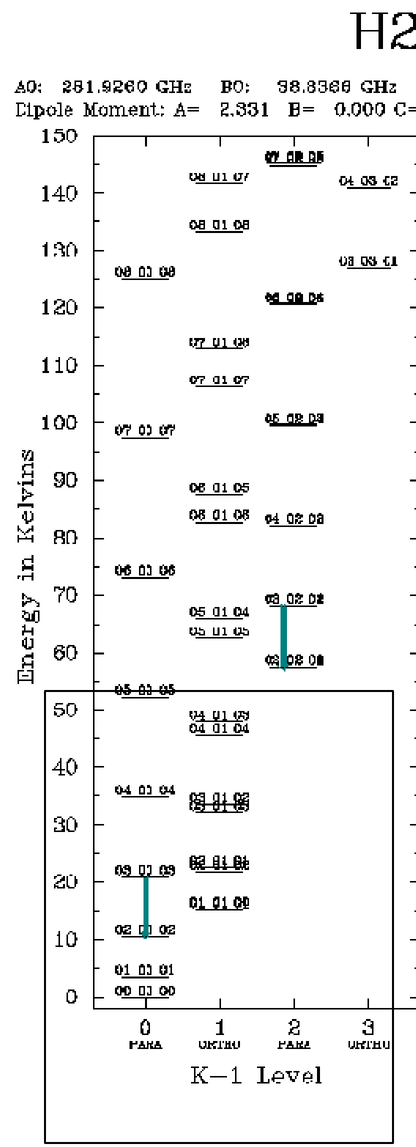
- Slightly asymmetric rotors
  - e.g. H_2CO
    - Many lines at nearly any frequency
    - Fewer within GBT range owing to its low weight
    - ^{13}C, ^{18}O, ^{17}O, HDCO, D_2CO available (and seen)
- Isotopic variants
  - Degrees of optical depth
    - CO—low dipole moment and abundant, so high optical depth, thermalized line useful for temperature measurements
    - HCO^+ --abundant ion, high dipole moment, often optically thick with several isotopes
    - CS, HCN, etc.
  - Chemical interest
    - Deuterated isotopomers



Formaldehyde, an asymmetric rotor molecule, has many transitions. Some of these, at different energy levels, lie adjacent in frequency and may be observed simultaneously.

One useful grouping of lines includes lines at 211, 218.2, 218.5, 218.8 and 226 GHz. The cluster at 218 GHz is especially well suited to existing correlators.

Furthermore, these lines lie at 23 K (218.2 GHz line) and 64 K (218.5; 218.8 GHz lines) above ground (nearly the same as ammonia), and are from the para form of formaldehyde.



Quantum Numbers J K−1 K1			Level Degeneracy	Energy Above Ground (Kelvins)
00	00	00	3.0	0.000
01	00	01	3.0	3.486
02	00	02	5.0	10.484
01	01	01	9.0	15.164
01	01	00	9.0	15.395
03	00	03	7.0	20.957
02	01	02	15.0	21.923
02	01	01	15.0	22.618
03	01	03	21.0	32.060
03	01	02	21.0	33.450
04	00	04	9.0	34.905
04	01	04	27.0	45.571
04	01	03	27.0	47.888
05	00	05	11.0	52.314
02	02	01	5.0	57.610
02	02	00	5.0	57.612
05	01	05	33.0	62.454
05	01	04	33.0	65.929
03	02	02	7.0	68.095
03	02	01	7.0	68.112
06	00	06	13.0	73.166
04	02	03	9.0	82.073
04	02	02	9.0	82.124
06	01	06	39.0	82.703
06	01	05	39.0	87.566
07	00	07	15.0	97.443
05	02	04	11.0	99.540
05	02	03	11.0	99.659
07	01	07	45.0	106.314
07	01	06	45.0	112.795
06	02	05	13.0	120.493
06	02	04	13.0	120.791
08	00	08	17.0	125.121
03	03	01	9.0	126.957
08	01	08	51.0	133.201
04	03	02	27.0	140.941
08	01	07	51.0	141.606
07	02	06	15.0	144.928
07	02	05	15.0	145.355

H_2CO at Low Frequencies

- Doubling within each K ladder produces lower frequency lines for density measurement
  - For K=1 lines at 6cm, 2cm, 1cm, 7mm, 3.3mm
  - K=2 lines unreported in literature, may be detectable at even lower frequencies
  - K=0 fundamental line at 72 GHz, close to 3.3mm K=1 line.
  - *Requires good calibration of intensity scale, pointing*
- Ideally, many lines can be measured and some disentanglement of structure along the line of sight can be accomplished
- D_2CO, HDCO as well as other isotopes seen

Examples

- DR21(OH)—a hot dense cloud with multiple star-forming cores
  - Ammonia, Formaldehyde, Methyl Cyanide
- IRAS16293-2422—cool cloud forming a low mass star
  - Ammonia, Formaldehyde
- Note that abundance may vary strongly, molecules may freeze onto grains at high density and low temperature, but the process may reverse near the star where temperatures rise.

DR21(OH)

H_2CO

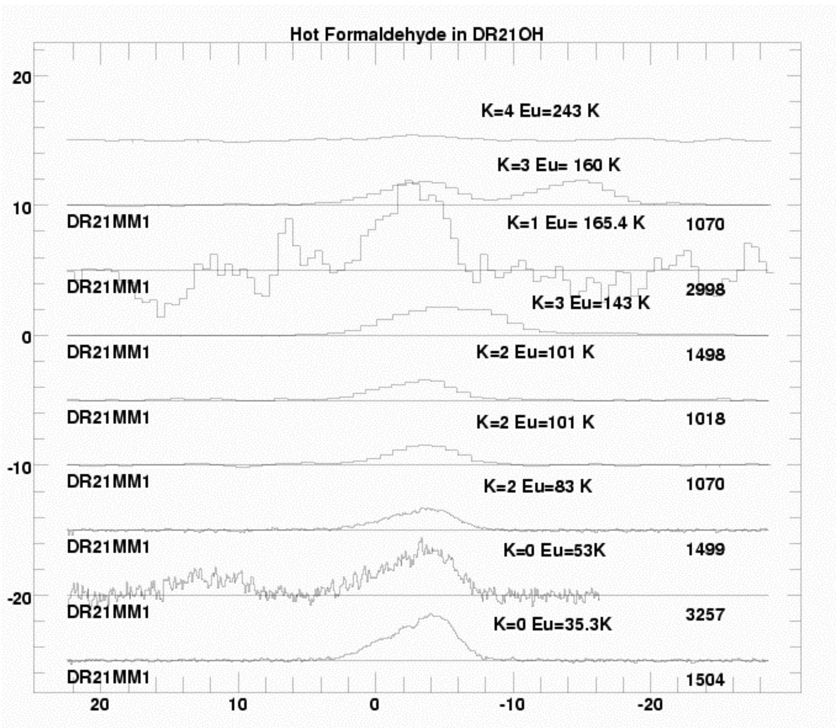
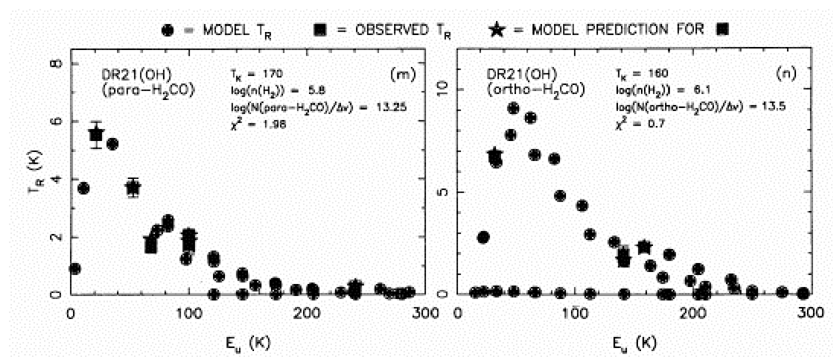


TABLE 1

Observed H_2CO Transitions

Transition	Frequency[a] (GHz)	Energy$_u$ (K)	θ_{mb}('')	η_{mb}
$4_{04} \rightarrow 3_{03}$	290.623405	35.0	24	0.7
$4_{23} \rightarrow 3_{22}$	291.237780	82.2	24	0.7
$4_{32} \rightarrow 3_{31}$	291.380488	141.1	24	0.7
$4_{31} \rightarrow 3_{30}$	291.384264	141.1	24	0.7
$5_{24} \rightarrow 4_{23}$	363.945894	99.6	19	0.64
$5_{42} \rightarrow 4_{41}$	364.103249	240.9	19	0.64
$5_{41} \rightarrow 4_{40}$	364.103249	240.9	19	0.64
$5_{33} \rightarrow 4_{32}$	364.275141	158.5	19	0.64
$5_{32} \rightarrow 4_{31}$	364.288884	158.5	19	0.64
$5_{23} \rightarrow 4_{22}$	365.363428	99.7	19	0.64
$9_{19} \rightarrow 8_{18}$	631.702813	163.73	12	0.32

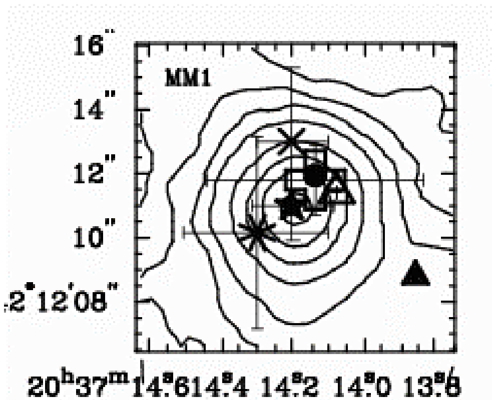
[a] Frequencies from Bocquet et al. 1996 *J. Mol. Spec.*, **177**, 154.

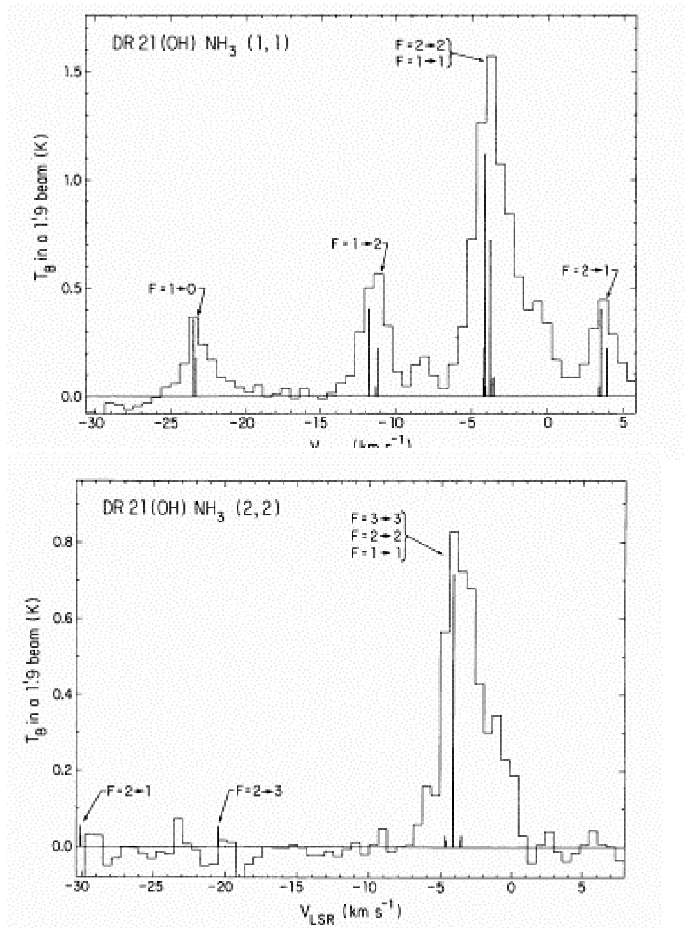


Note velocity shifts with 🖫 -- two sources!

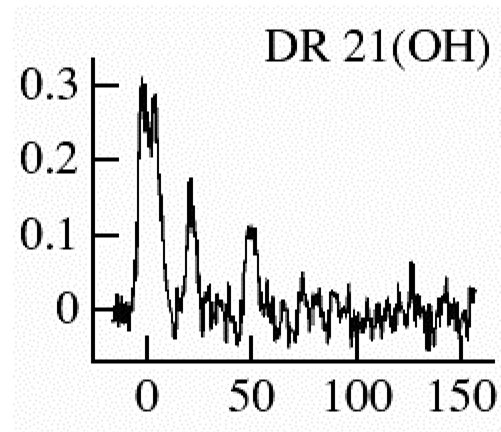
DR21(OH)

Interferometric NH_3



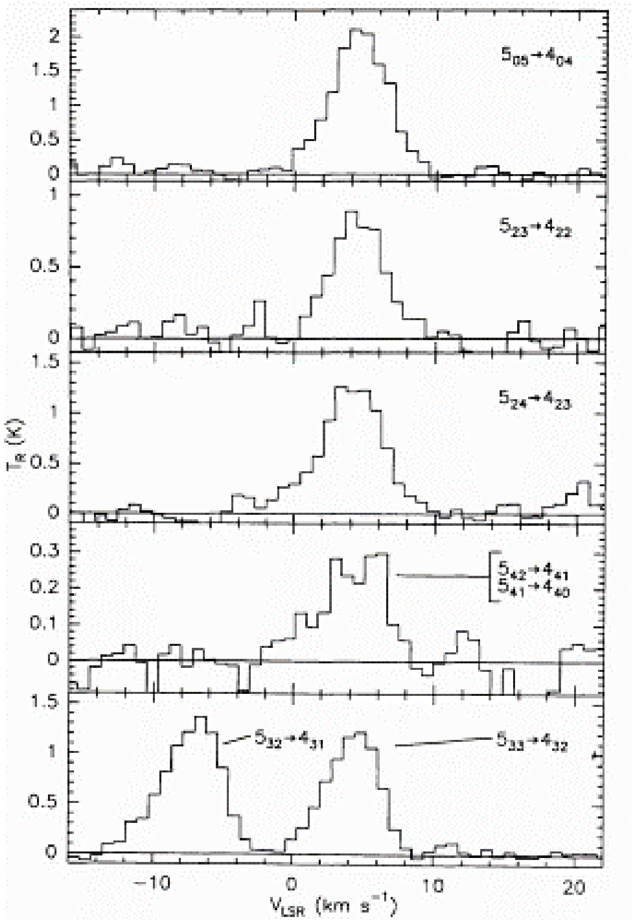


CH_3CN $J_K=6_K-5_K$

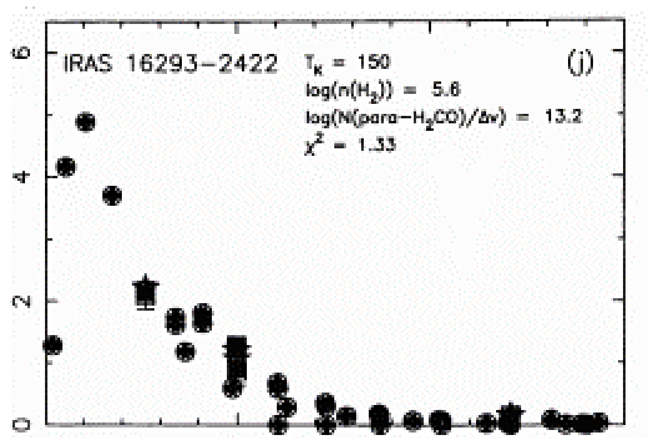


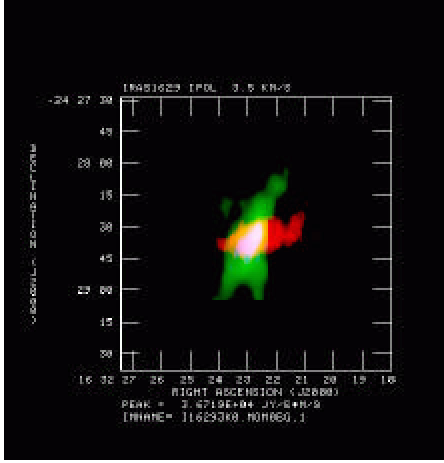
IRAS16293

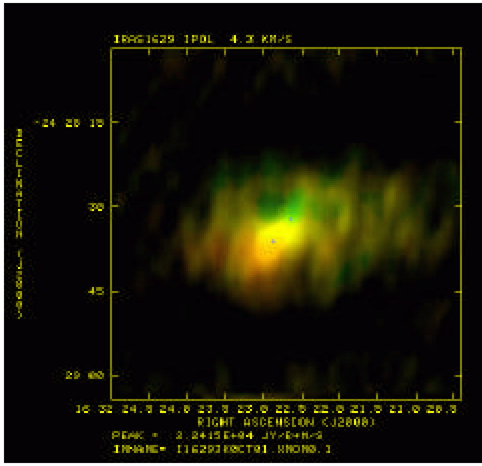
H_2CO

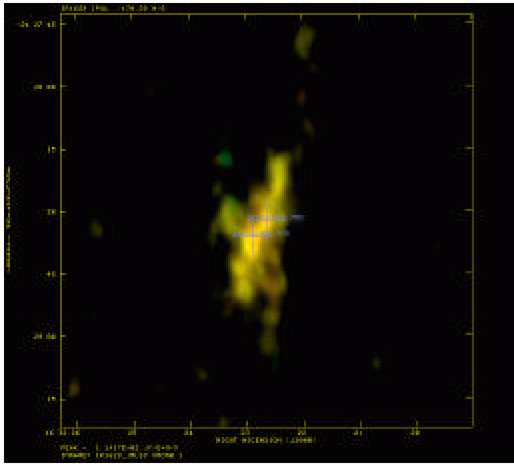


Intermediate mass young Binary, still accreting matter From its surrounding core ~30 L_{sun} T_k~50 K.



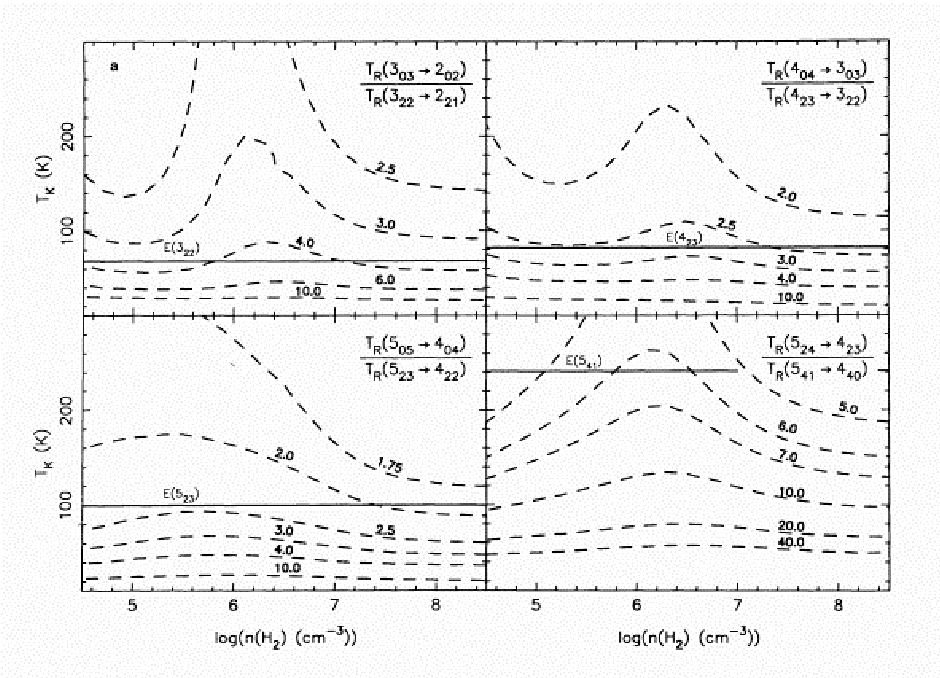




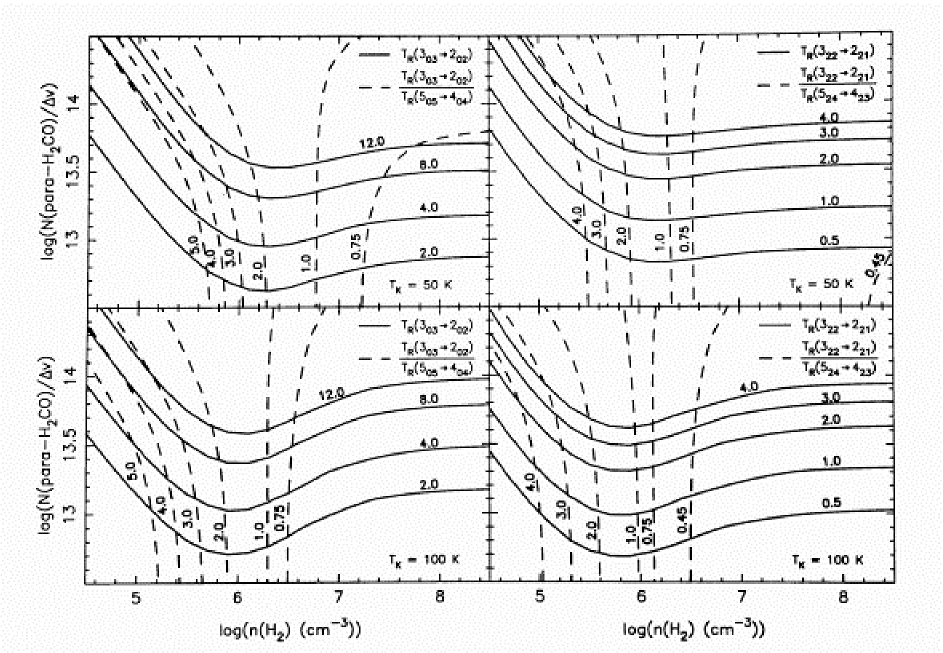


H_2CO Model Grids

Kinetic Temperature



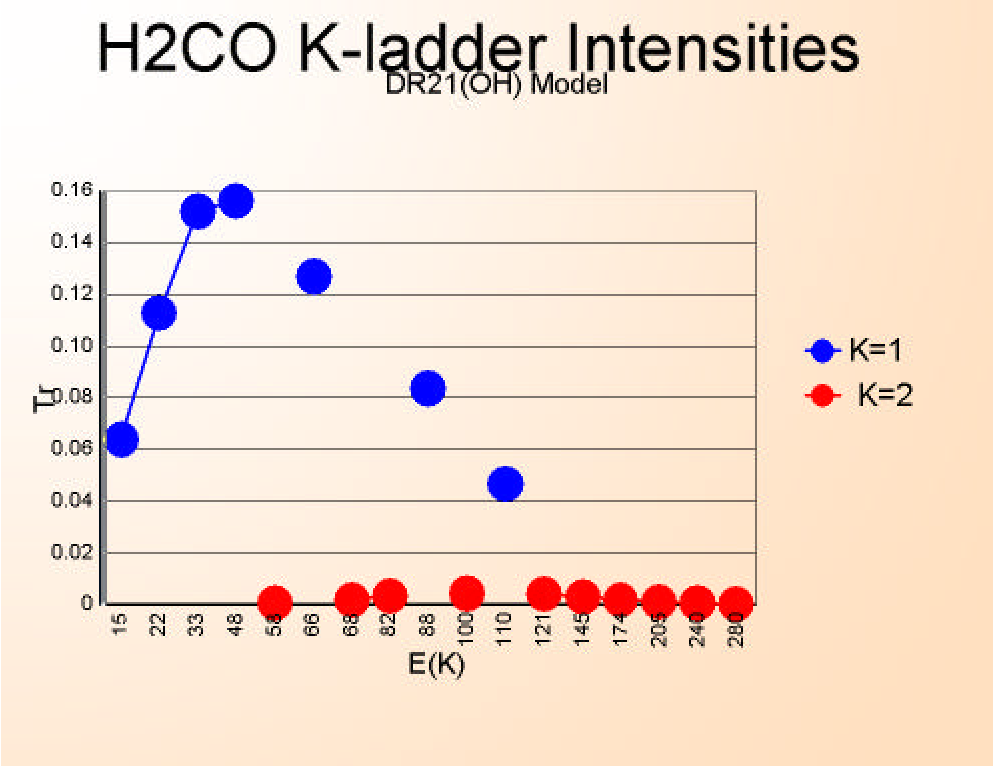
Density



Note that the ratio measured varies rapidly and quasi-linearly with the quantity to be measured.

H_2CO Transitions for cm wavelengths

- K-doublet transitions within the K=1 and K=2 ladders lie within cm frequency range
- K=2 K-doublets not reported but should be within reach
- Should provide good density probe for dense regions with sufficient column density.



Chemistry

- Study of relative abundances can give important clues to abundances of unobserved species
- Example—how is it that we can observe ND_3 and D_2CO?
- Some broad brush points about chemistry
  - Space is empty! The collision frequency is low (once every two weeks for a moderately dense region ($n \sim 10^4$ cm^{-3})
  - To be important, a reaction must ‘go’ at every collision
  - Clouds are cold—no energy barriers!
    - Stronger bonds are favored
  - Coulomb interactions favored
    - Higher collision cross section
    - Higher potential for interaction
  - Ion Molecule chemistry has been the paradigm
    - Charge transfer reactions
    - Exchange reactions
    - Recombination

Example—Deuterium Enhancement

- Basic ion-molecule reaction
- Among best-tested reaction network
  - Involves basic, observable molecules
  - Several variants
  - Many within GBT-mm frequency range
- Normally, isotopic variants, particularly when the variant is D, lie moderately far in frequency from the abundant variety
  - Good brightness temperature calibration essential
  - Good pointing performance
  - Good sensitivity? After all, [D]/[H]~ few x 10^{-5} in SMOW (Standard Mean Ocean Water).

Deuterium Fractionation

Of particular importance are exchange reactions, of the type:

$$AH^+ + HD \leftrightarrows AD^+ + H_2 + \Delta E \, .$$

Proceeding at rate k_2, and which only occurs for some particular species A; in particular for A=H_2:

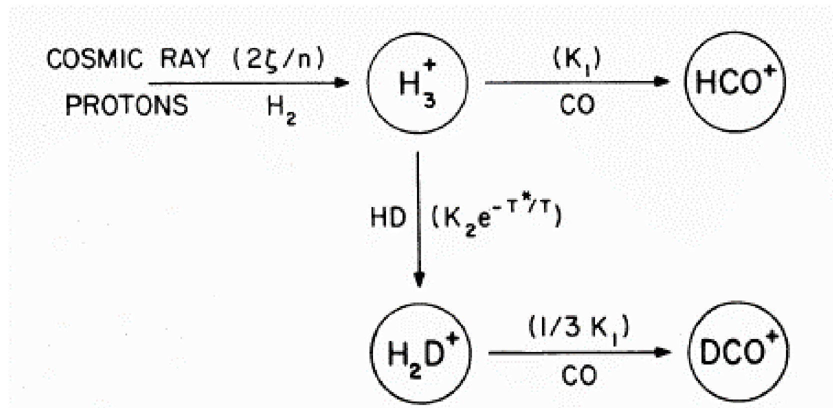
$$\Delta E / k \sim 180 \text{ K}$$

And thus this reaction tends to enhance H_2D^+ in cold regions. To estimate the Amount of enhancement, we assume equilibirium—that is that the destruction rate equals the creation rate—and solve for the enhancement ratio. What destroys H_3^+ in space? Since it is a cornerstone molecule, most simple molecules *i* react with it at rate k_i. It is also destroyed by the reverse of the exchange reaction above, and by recombination with electrons. Solving,

$$R' = \frac{x(AD^+)}{x(AH^+)} < \frac{4 \times 10^{-5} k_2}{10^{-6} x_e + k_2 \exp\left(-\Delta E / kT\right) + \Sigma k_i x_i} \, .$$

Example—Deuterium Enhancement

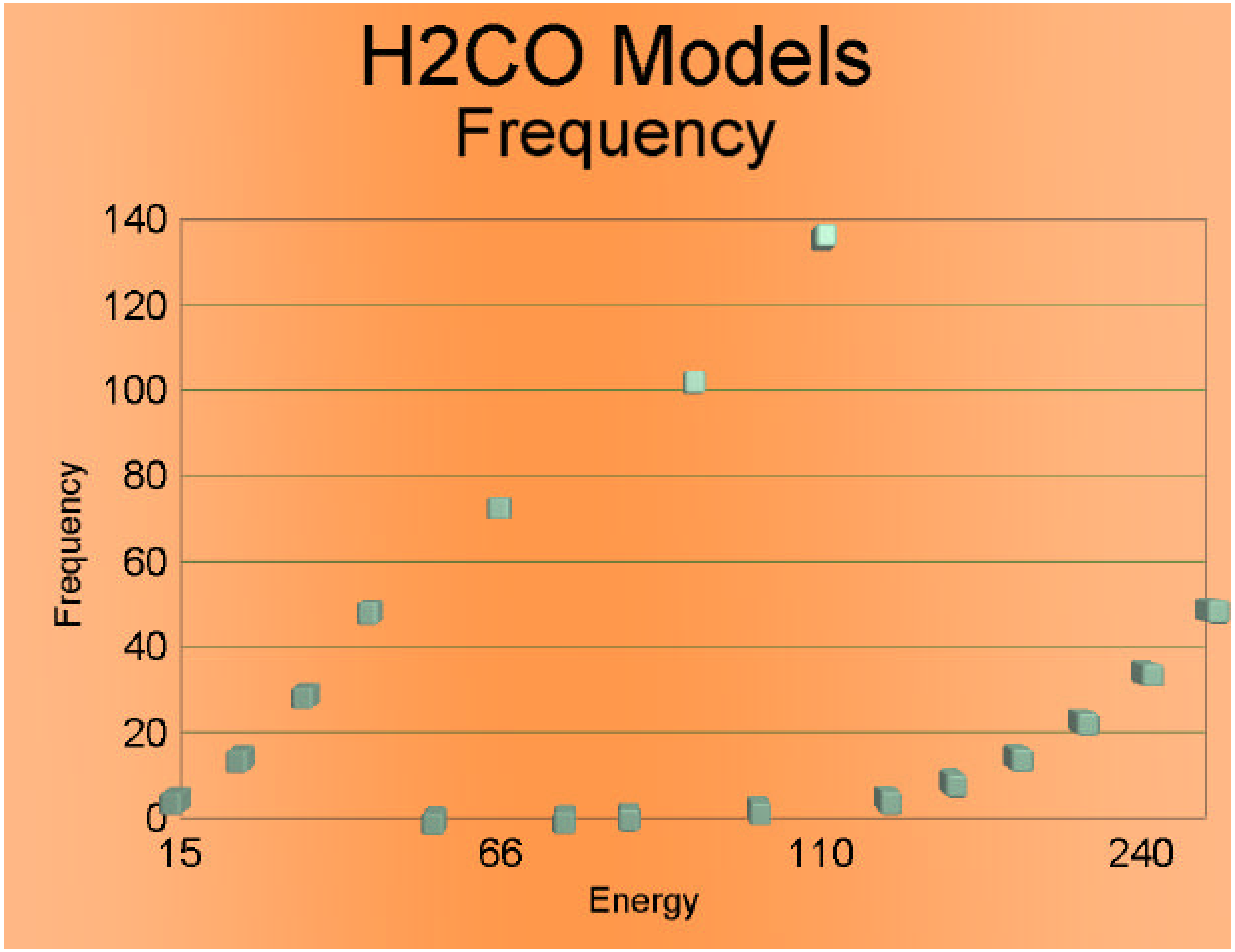
- Observed ratios, R~0.05-0.10, suggest $x_e<10^{-8}$, $x_{CO}\sim10^{-5}$, T<20K…
- Surprisingly, recently in the coldest and densest clouds, ND_3 D_2CO H_2D^+ and perhaps D_2H^+ have been found with surprisingly strong emission
- Such a major unaccounted D-reservoir may affect D, HD abundances in the interstellar medium at large.



$$\frac{x(\mathrm{HCO^+})}{x(\mathrm{CO})} = \frac{[2\zeta/n(\mathrm{H_2})]K_1}{(\beta x_e + \delta)(\beta' x_e + \delta')}\,, \qquad (1)$$

$$R \equiv \frac{x(\mathrm{DCO^+})}{x(\mathrm{HCO^+})} = \frac{\frac{1}{3}x(\mathrm{HD})K_2}{K_2 \exp(-T^*/T) + (\beta x_e + \delta)}\,. \qquad (2)$$

The End


H2CO Models
Frequency
Frequency
140
120
100
80
60
40
20
0
15
66
110
240
Energy

The Interstellar Molecular Zoo By Number of Atoms

H_2	C_3	$c\text{-}C_3H$	C_5	C_5H	C_6H	CH_3C_3N	CH_3C_4H	CH_3C_5N	HC_9N	$HC_{11}N$
AlF	C_2H	$l\text{-}C_3H$	C_4H	$l\text{-}H_2C_4$	CH_2CHCN	$HCOOCH_3$	CH_3CH_2CN	$(CH_3)_2CO$		C_6H_6?
AlCl	HCN	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH	$(CH_3)_2O$	NH_2CH_2COOH?		
C_2	C_2O	C_3O	$l\text{-}C_3H_2$	CH_3CN	HC_5N	C_7H	CH_3CH_2OH			
CH	C_2S	C_3S	$c\text{-}C_3H_2$	CH_3NC	$HCOCH_3$	H_2C_6	HC_7N			
CH^+	CH_2	C_2H_2	CH_2CN	CH_3OH	NH_2CH_3	CH_2OHCHO	C_8H			
CN	HCO	CH_2D^+	CH_4	CH_3SH	$c\text{-}C_2H_4O$					
CO	HCO^+	HCCN	HC_3N	HC_3NH^+	CH_2CHOH					
CO^+	HCS^+	$HCNH^+$	HC_2NC	HC_2CHO						
CP	HOC^+	HNCO	HCOOH	NH_2CHO						
CSi	H_2O	HNCS	H_2CHN	C_5N						
HCl	H_2S	$HOCO^+$	H_2C_2O							
KCl	HNC	H_2CO	HC_3N							
NH	HNO	H_2CN	H_2NCN							
NO	MgCN	H_2CS	H_2COH^+							
NS	MgNC	H_3O^+	SiH_4							
NaCl	N_2H^+	NH_3								
OH	N_2O	SiC_3								
PN	NaCN	CH_3								
SO	OCS									
SO^+	SO_2									
SiN	$c\text{-}SiC_2$									
SiO	CO_2									
SiS	NH_2									
HF	H_3^+									
FeO	H_2D^+									
CS										