



Status of Spectral Line Catalogs

Line Identification Data for Herschel, ALMA and SOFIA

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Existing Microwave Catalogs

- ◆ **Microwave Catalogs (better than 100kHz accuracy if in range of available data)**
 - **JPL Microwave, Millimeter and Submillimeter Spectral Line Catalog**
 - <http://spec.jpl.nasa.gov>
 - Pickett et al., 1998, J. Quant. Spec. & Rad. Transfer 60, 883.
 - Fitting programs provided on line
 - 340+ entries
 - **CDMS Cologne Database for Molecular Spectroscopy**
 - <http://www.ph1.uni-koeln.de/vorhersagen/>
 - H. S. P. Müller et al., 2005, J. Mol. Struct. 742, 215-227
 - 380+ entries
 - **NIST**
 - **Recommended Rest Frequencies**
 - <http://physics.nist.gov/cgi-bin/micro/table5/start.pl>
 - Lovas, 1992, J. Phys. Chem. Ref. Data 21, 181.
 - **J. Phys. Chem. Ref. Data Historical data**
 - <http://www.physics.nist.gov/PhysRefData/MolSpec/Diatomic/index.html>
 - <http://www.physics.nist.gov/PhysRefData/MolSpec/Hydro/index.html>
 - <http://www.physics.nist.gov/PhysRefData/MolSpec/Triatomic/index.html>



Existing Line Resolved IR Catalogs

◆ Line Resolved Infrared Catalogs (Accuracy of 3-30 MHz)

- HITRAN “high-resolution transmission molecular absorption database”
 - 39 Mostly Atmospheric Molecules
 - <http://cfa-www.harvard.edu/HITRAN/>
 - Rothman, L.S., 2005, JSQRT 96, 139
- GEISA Gestion et Etude des Informations Spectroscopiques Atmosphériques
 - 42 Mostly Atmospheric Molecules
 - <http://ara.lmd.polytechnique.fr>
 - Jacquinet-Husson et al., 2003, *Atmos. Oceanic Opt.* ,16-3, 256-61.
- NIST (Better than 3 MHz)
 - Heterodyne IR spectra of 5 molecules
 - <http://physics.nist.gov/PhysRefData/wavenum/html/contents.html>
 - Maki, A. G. and Wells, J. S. (1998), *Wavenumber Calibration Tables from Heterodyne Frequency Measurements* (version 1.3).



Other Data and Data Bases

- ◆ **No Astrophysical Molecular Database of IR or Optical/UV**
 - Few molecules have known IR spectrum (only simple)
 - Few molecules have known electronic spectrum (only simple)
 - Many notable surprises (electronic bands of HCO+!)

- ◆ **Far IR often lacks even band data**
 - Few spectra from 3-400 cm^{-1} of more complex molecules
 - Applies to liquid and gas

- ◆ **Basic rotational information is collected**
 - <http://www.uni-ulm.de/strudo/mogadoc/>
 - Fee \$\$, collection of references and constants
 - No critical evaluation



Catalog Support

- ◆ **IR catalogs supported by atmospheric science community**
 - HITRAN is actively supported
 - Latest review meeting June 2006
 - GEISA also appears actively supported (CNES in France)

- ◆ **Microwave catalogs support both Astronomy and Atmospheric Science**
 - JPL is funded only by atmospheric science as part of Aura validation
 - No Astrophysics funding since 2000
 - Some Herschel money (2007, 2008)
 - CDMS dedicated to astrophysics
 - Funding expired in 2005
 - ESA did not honor commitment to fund 2005-Herschel Launch
 - MPIfR/DLR are currently supporting CDMS
 - NIST is not funded Frank Lovas supports in his spare time

- ◆ **JPL and CDMS are both used by Herschel observation planning tool HSPOT**

- ◆ **NASA Laboratory Astrophysics Workshop (Feb 2006) supported data generation over catalogs**



Known Molecules

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms	9 atoms	10 atoms	11 atoms	12 atoms	13 atoms
H ₂	C ₃ *	c-C ₃ H	C ₅ *	C ₅ H	C ₆ H	CH ₃ C ₃ N	CH ₃ C ₄ H	CH ₃ C ₅ N	HC ₉ N	C ₆ H ₆ * (?)	HC ₁₁ N
AlF	C ₂ H	l-C ₃ H	C ₄ H	l-H ₂ C ₄	CH ₂ CHCN	HCOOCH ₃	CH ₃ CH ₂ CN	(CH ₃) ₂ CO	CH ₃ C ₆ H	C ₂ H ₅ OCH ₃ (?)	
AlCl	C ₂ O	C ₃ N	C ₄ Si	C ₂ H ₄ *	CH ₃ C ₂ H	CH ₃ COOH	(CH ₃) ₂ O	(CH ₂ OH) ₂			
C ₂ **	C ₂ S	C ₃ O	l-C ₃ H ₂	CH ₃ CN	HC ₅ N	C ₇ H	CH ₃ CH ₂ OH	CH ₃ CH ₂ CHO			
CH	CH ₂	C ₃ S	c-C ₃ H ₂	CH ₃ NC	CH ₃ CHO	H ₂ C ₆	HC ₇ N				
CH ⁺	HCN	C ₂ H ₂ *	H ₂ CCN	CH ₃ OH	CH ₃ NH ₂	CH ₂ OHCHO	C ₈ H				
CN	HCO	NH ₃	CH ₄ *	CH ₃ SH	c-C ₂ H ₄ O	l-HC ₆ H* (?)	CH ₃ C(O)NH ₂				
CO	HCO ⁺	HCCN	HC ₃ N	HC ₃ NH ⁺	H ₂ CCHOH	CH ₂ CHCHO (?)					
CO ⁺	HCS ⁺	HCNH ⁺	HC ₂ NC	HC ₂ CHO		CH ₂ CCHCN					
CP	HOC ⁺	HNCO	HCOOH	NH ₂ CHO							
SiC	H ₂ O	HNCS	H ₂ CNH	C ₅ N							
HCl	H ₂ S	HOCO ⁺	H ₂ C ₂ O	l-HC ₄ H* (?)							
KCl	HNC	H ₂ CO	H ₂ NCN	l-HC ₄ N							
NH	HNO	H ₂ CN	HNC ₃	c-H ₂ C ₃ O							
NO	MgCN	H ₂ CS	SiH ₄ *	H ₂ CCNH (?)							
NS	MgNC	H ₃ O ⁺	H ₂ COH ⁺								
NaCl	N ₂ H ⁺	c-SiC ₃									
OH	N ₂ O										
PN	NaCN										
SO	OCS										
SO ⁺	SO ₂										
SiN	c-SiC ₂										
SiO	CO ₂ *										
SiS	NH ₂										
CS	H ₃ ⁺										
HF	H ₂ O ⁺										
SH [*]	SiCN										
HD	AlNC										
FeO (?)	SiNC										
O ₂ (?)											
CF ⁺											
SiH (?)											

Note: Many simple molecules necessary for Chemical network to function have not yet been Observed e.g. NH⁺, NH₂⁺, NH₃⁺, OH⁺, CH₂⁺, CH₃, CH₃⁺



Known diatomics

◆ Diatomics (Main isotope name given)

- Known Molecules H_2 , AlF, AlCl, C_2 , CH, CH⁺, CN, CO, CO⁺, CP, CSi, HCl, KCl, NH, NO, NS, NaCl, OH, PN, SO, SO⁺, SiN, SiO, SiS, CS, HF, SH, FeO, O₂, CF⁺, SiH
 - Red = nothing in catalog
- Dunham Theory allows isotopes and vibrations to be calculated together if enough data exists on one or more isotopic species
- Catalogs contain all but one known and many unknown diatomics
- Needs mass independent fits for many, many species have no vibrational information (e.g. CO)
- Additional transition metal hydrides and oxides probably should be cataloged



Status Known Diatomics (1/2)

Molecule	V's	N, Freq	Isotopes	V's	N, Freq	JPL	CDMS	
H ₂	None		HD	V=0	J=1 2.6 THz	Yes	Yes	
AlF	V=0	N=14 461 GHz	None			Yes		
AlCl-35	V=0	N=1 15 GHz	AlCl-37	V=0	N=1 15 GHz	Yes		
C ₂	None	No Dipole	None					
CH	V=0	N=8 4.2 THz	None			Yes	Yes	CD data at JPL
CH+	V=0	J=1 835 GHz	None			Yes		CD+/13CH+ being done at JPL
CN	V=0,1	N=8 1THz	13CN	V=0	N=2 217 GHz	Yes	Yes	
			C15N	V=0	N=2 219 GHz		Yes	
			13C15N	V=0	predictions		Yes	
CO	V=0	J=38 4.3 THz	13CO	V=0	J=30 3.3 THz	Yes	Yes	Data Available for V>0
			C18O	V=0	J=18 2 THz	Yes	Yes	Data Available for V>0
			C17O	V=0	J=8 900 GHz	Yes	Yes	Data Available for V>0
			13C18O	V=0	J=9 1 THz		Yes	
			13C17O	V=0	J=9 1 THz		Yes	
CO ₂	V=0	N=4 471 GHz	None			Yes		Data Available to N=5 Arizona
CP	V=0	N=22 1 THz	None			Yes	Yes	
SiC	V=0,1	N=12 460 GHz	Si13C	V=0	N=8 270 GHz	Yes	Yes	
			29/30SiC					
HCl-35	V=0	N=10 6.2 THz	HCl-37	V=0	N=10 6.2 THz	Yes		
			DCl-35	V=0	N=2 646 GHz	Yes		
			DCl-37	V=0	N=2 645 GHz	Yes		
KCl-35	V=0,1	N=134 930 GHz	KCl-37	V=0,1	N=138 925 GHz	Yes	Yes	
			41K35Cl	V=0,1	N=134 908 GHz		Yes	
			41K37Cl					Can calculate
NH	V=0	N=5 4.9 THz	ND	V=0	N=2 1.1 THz	Yes	Yes	
			15NH					
NO	V=0,1	N=6 464 GHz	None			Yes		
NS	V=0	N=8 350 GHz	N34S	V=0	N=3 115 GHz	Yes		
			15NS					
NaCl-35	V=0,1	J=73, 930 GHz	NaCl-37	V=0,1	J=74, 930 GHz	Yes	Yes	
OH	V=0-2	N=9 3.8 THz	OD	V=0	N=11 2.5 THz	Yes		3 MHz accuracy
			18OH	V=0	N=3 6 GHz	Yes		
			18OD					
			17OH					



Status Known Diatomics (2/2)

Molecule	V's	N, Freq	Isotopes	V's	N, Freq	JPL	CDMS	
PN	V=0-4	N=8 375 GHz	None			Yes		
SO	V=0,1	N=44 1.9 THz	33SO	V=0	N=24 1 THz	Yes	Yes	also a state
			S17O	V=0	N=15 620 GHz		Yes	
			34SO	V=0	N=25 1 THz	Yes	Yes	
			S18O	V=0	N=26 1 THz	Yes	Yes	
			36SO	V=0	N=23 952 GHz		Yes	
			Doubles					Can calculate all
SO+	V=0	N=7 350 GHz	None					
SiN	V=0	N=4 178 GHz	None					
SiO	V=0-6	N=8 340 GHz	29SiO	V=0-3	N=1 43 GHz	Yes	Yes	
			30SiO	V=0-3	N=1 43 GHz		Yes	
			Si18O	V=0-3	N=11 444 GHz		Yes	
			Si17O					Needed to calculate all
SiS	V=0	N=3 55 GHz	29SiS	V=0	N=3 55 GHz	Yes		
			30SiS	V=0	N=3 55 GHz	Yes		
			Si34S	V=0	N=3 55 GHz	Yes		
			Si33/36S					Needed to calculate all
CS	V=0-2	N=22 1.1 THz	13CS	V=0,1	N=22 1 THz	Yes	Yes	
			C33S	V=0,1	N=22 1 THz		Yes	
			C34S	V=0,1	N=22 1 THz	Yes	Yes	
			13C33S	V=0	N=20 1 THz		Yes	
			13C34S	V=0	N=21 1 THz		Yes	
			C36S	V=0	N=21 1 THz		Yes	
			13C36S	V=0			Yes	Calculated
HF	V=0	N=5 6.2 THz	DF	V=0	N=1 652 GHz	Yes		
SH	V=0,1	N=5 875 GHz	SD	V=0	N=6 1 THz	Yes		
			33/34/36SH					Needed to calculate all
FeO			None					Some data exists
O2	V=0,1	N=15 2.5 THz	O17O	V=0	N=1 118 GHz	Yes		also Delta state
			O18O	V=0	N=3 463 GHz	Yes		
CF+	V=0,1	N=4 411 GHz	None				Yes	
SiH			None					



Diatomic Work Remaining

- ◆ AIF should be extended to 1 THz (ALMA primary)
- ◆ AlCl (³⁵Cl and ³⁷Cl) should be extended to 500 GHz (ALMA primary)
- ◆ CO calculation of V=1 for all needed (data is available)
- ◆ ¹³CN, C¹⁵N and ¹³C¹⁵N should be extended to 2 THz (Herschel)
- ◆ CO⁺ should be extended to 2 THz (Herschel)
 - ¹³CO⁺, C¹⁷O⁺, C¹⁸O⁺ should be measured to 2 THz
 - Double versions can then be calculated
- ◆ ¹³CP should be measured to 1 THz (ALMA)
- ◆ ⁴¹K³⁷Cl should be calculated (can be done from existing data) (ALMA)
- ◆ SiC should be extended to 2 THz (Herschel)
 - ²⁹SiC, ³⁰SiC, Si¹³C should be measured to 2 THz
 - Double substituted can then be calculated
- ◆ ¹⁵NH needs to be measured (Herschel)
 - ¹⁵ND should be calculated once ¹⁵NH is measured
- ◆ ¹⁸OH, ¹⁷OH need to have rotational transitions measured (Herschel)
 - ¹⁸OD and ¹⁷OD can then be calculated
- ◆ PN should be extended to 1 THz (ALMA)
 - P¹⁵N should be measured to 1 THz
- ◆ SO should be extended to 2 THz and V=3 (Herschel, ALMA)
 - Mixed isotopes should be calculated
- ◆ SO⁺ should be extended to 2 THz and V=1
 - Isotopes ³³S, ³⁴S, ³⁶S, ¹⁷O and ¹⁸O should be measured
 - Mixed isotopes can then be calculated
- ◆ SiN should be extended to 2 THz and V=1
 - ²⁹Si, ³⁰Si, ¹⁴N should be measured to 2 THz
 - Mixed isotopes can then be calculated
- ◆ SiO should be extended to 2 THz
 - ²⁹Si, ³⁰Si, ¹⁸O need to be extended
 - ¹⁷O needs to be measured
 - Mixed isotopes can then be calculated
- ◆ SiS should be extended to 500 GHz
 - ²⁹Si, ³⁰Si, ³³S, ³⁴S, ³⁶S should be measured/extended
 - Mixed isotopes can then be calculated
- ◆ SH should be extended to 2 THz
 - ³³S, ³⁴S, ³⁶S should be measured
 - Mixed isotopes can then be calculated
- ◆ FeO need to be cataloged and evaluated
 - Most likely ¹⁷O and ¹⁸O need to be measured
- ◆ CF⁺ should be extended to 2 THz
 - ¹³CF⁺ should be measured
- ◆ ¹³CH and CD need to be measured
- ◆ ¹³CH⁺ and CD⁺ need to be measured
- ◆ SiH, SiD, ²⁹SiH, ³⁰SiH need to be measured/evaluated
 - Mixed versions can then be calculated



Known triatomics

◆ Triatomics

- **Known Molecules** C_3 , C_2H , C_2O , C_2S , CH_2 , HCN , HCO , HCO^+ , HCS^+ , HOC^+ , H_2O , H_2O^+ , H_2S , HNC , HNO , $MgCN$, $MgNC$, N_2H^+ , N_2O , $NaCN$, OCS , SO_2 , $c-SiC_2$, CO_2 , NH_2 , H_3^+ , $SiCN$, $SiNC$, $AlNC$
 - **Red=Nothing in Catalog**
- **Catalogs contains most known and a few unknown triatomics**
- **Each isotopomer and vibrational state is a separate spectroscopic problem**
- **Vibrational data is scarce**
- **Isotopic data is lacking on many species**



Status known triatomics (1/2)

3 atom molecules								
Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
C ₃	nu ₂	14, 2 THz	None				Yes	No rotation spectrum
C ₂ H	nu ₂	11, 960/350	CCD	V=0	5, 360 GHz		Yes	
			13CCH	V=0	4, 336 GHz		Yes	
			C13CH	V=0	4, 341 GHz		Yes	
C ₂ O	V=0	8, 185 GHz	None			Yes		
C ₂ S	V=0	23, 285 GHz	None			Yes	Yes	
CH ₂	V=0	5, 1 2 THz	None				Yes	Cannot extrapolate
HCN	nu ₂	22, 2 THz	DCN	nu ₂	27, 2 THz		Yes	
			H13CN	nu ₂	23, 2 THz		Yes	
			HC15N	nu ₂	23, 2 THz		Yes	
			D13CN	V=0	29, 2 THz		Yes	
			DC15N	V=0	28, 2 THz		Yes	
			H13C15N					
			D13C15N	V=0	29, 2 THz		Yes	
HCO	V=0	11, 1, 360 GHz	None			Yes		
HCO ⁺	000,010,020 100,001	12, 1 THz	DCO ⁺	V=0	11, 792 GHz	Yes	Yes	Paper in press, DCO+ vib data
			H13CO ⁺	V=0	3, 260 GHz	Yes	Yes	Paper in press JPL/CESR
			HC18O ⁺	V=0	3, 255 GHz	Yes	Yes	Paper in press JPL/CESR
			HC17O ⁺	V=0	4, 370 GHz	Yes	Yes	
			D13CO ⁺	V=0	11, 778 GHz		Yes	Paper in press JPL/CESR
			DC18O ⁺	V=0	10, 689 GHz		Yes	Paper in press JPL/CESR
HCS ⁺	V=0	23, 940 GHz	DCS ⁺	V=0	26, 936 GHz		Yes	
			H13CS ⁺	V=0	9, 367 GHz		Yes	
			HC34S ⁺	V=0	21, 881 GHz		Yes	
			33S,36S					
HOC ⁺	nu ₂	9, 813 GHz	DOC ⁺	V=0	11, 840 GHz		Yes	
			H013C⁺					
			H180C⁺					
H ₂ O	nu ₁ , nu ₂ , nu ₃ 2nu ₂	17, 9, 5.6 THz	HDO	V=0	12, 7 2 THz	Yes		Data Cologne, JPL
			H218O	V=0	7, 4 750 GHz	Yes		More data available in GS
			H217O	V=0	7, 3 750 GHz	Yes		No hyperfine, GS data available
			D2O	V=0	12, 10 1 THz	Yes		Paper in press
			HD18O	V=0	12, 5 241 GHz	Yes		Data at JPL, Caltech
			HD17O					Some data is available
			D218O					Some data is available
			D217O					Some data is available
H ₂ S	V=0	13, 9, 1 THz	HDS	V=0	12, 6 630 GHz	Yes		
			33/34/36S					



Status known triatomics (2/2)

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
HNC	nu2	22, 2 THz	DNC	V=0	26, 2 THz		Yes	
			H13CN	V=0	2, 180 GHz	Yes		
			HC15N	V=0	2, 180 GHz	Yes		
			doubles					
HNO	V=0	13,3, 490 GHz	DNO	V=0	10,3 375 GHz	Yes		
			15N,18O					
MgCN	V=0	37, 376 GHz	None			Yes		
MgNC	nu2	31, 375 GHz	None				Yes	
N2H+	nu2	8, 745 GHz	N2D+	V=0	9, 683		Yes	
			15NNH+	V=0	1, 91 GHz		Yes	
			N15NH+	V=0	1, 91 GHz		Yes	
NaO	nu2, 2nu2	66 1.7 THz	N218O		67, 1.7 THz	Yes		
			15NNO		67, 1.7 THz	Yes		
			N15NO		67, 1.7 THz	Yes		
NaCN	None	None	None					
OCS	V=0,1	90, 1090 GHz	O13CS	V=0	26, 315 GHz		Yes	
			18OCS	V=0	44, 501 GHz		Yes	
			OC34S	V=0	68, 805 GHz		Yes	
			17OCS	V=0	42, 504 GHz		Yes	
			OC33S	V=0	42, 504 GHz		Yes	
			O13C33S	V=0	42, 502 GHz		Yes	
			O13C34S	V=0	42, 496 GHz		Yes	
			18O13CS	V=0	60, 682 GHz		Yes	
			36S					
SO2	nu2	80,21 1.9 THz	33SO2	V=0	50,10, 1THz		Yes	
			S17O0	V=0	45,10, 1THz		Yes	
			34SO2	V=0	45,13, 1.2THz		Yes	
			S18O0	V=0	55,12, 1.2THz		Yes	
			36S					
c-SiC2	V=0	17,11, 369GHz	None			Yes		
CO2			C17O0	V=0	1, 22 GHz			No rotation spectrum in CO2
			C18O0	V=0	8, 176 GHz			
NH2	V=0	5,4,1.6 THz	None				Yes	
H3+			H2D+	V=0	3,2 1.4 THz	Yes	Yes	No rotation spectrum in H3+
			D2H+	V=0	2,2 1.5 THz		Yes	
H2O+	None	None	None					
SiCN	V=0	31, 338 GHz	None				Yes	
AlNC	V=0	32, 382 GHz	None				Yes	
SiNC	V=0	27, 340 GHz	None				Yes	



Tritomic Work Remaining

- ◆ C_3 requires single ^{13}C isotopes (2 possibilities)
- ◆ C_2H needs extending to 2 THz as do three isotopic versions
- ◆ C_2O needs to be extended to 1.5 THz and two ^{13}C and two O isotopes need to be done
- ◆ C_2S need to be extended to 1 THz and two ^{13}C and three S isotopes need to be done
- ◆ HCD and $H_2^{13}C$ need to be done
- ◆ HCN states below 5000cm^{-1} are needed, $^{13}C^{15}NH$ is needed
- ◆ HCO needs extending and isotopes (5) need to be done
- ◆ HCO^+ needs extending to 2 THz (7 total isotopes)
- ◆ $H^{13}CS^+$ needs extending, ^{33}S , ^{36}S need to be done
- ◆ ^{13}C and ^{18}O HOC^+ need to be done
- ◆ Nu1, 2nu2, nu3 water are needed, nu2 of ^{17}O and ^{18}O and double and triple substituted
- ◆ H_2S needs extending to higher J, HDS needs extending, isotopic S (3) is needed
- ◆ ^{13}C and ^{15}N HNC need extending, double substituted need to be done
- ◆ HNO and DNO need extending, ^{15}N , ^{17}O , ^{18}O need to be done
- ◆ MgNC needs to be extended, isotopes need to be done
- ◆ MgCN needs to be extended, isotopes need to be done
- ◆ N_2H^+ and 3 isotopes need extending
- ◆ 6 OCS isotopes need extending and 8 need $v=1$
- ◆ SiC_2 needs extending and isotopes need to be done
- ◆ Isotopic NH_2 needs to be done
- ◆ More H_2D^+ and D_2H^+ lines need to be measured
- ◆ H_2O^+ needs to be done as do isotopes
- ◆ SiNC, SiCN need extending and isotopes need to be done
- ◆ AINC needs to be extended and isotopes need to be done



Four atom molecules

◆ Four Atom Molecules

- Known Molecules $c\text{-C}_3\text{H}$, $l\text{-C}_3\text{H}$, C_3N , C_3O , C_3S , C_2H_2 , NH_3 , HCCN , HCNH^+ , HNCO , HNCS , HOCO^+ , H_2CO , H_2CN , H_2CS , H_3O^+ , $c\text{-SiC}_3$
 - Red= not in catalog
- Each isotopomer and vibrational state is a separate spectroscopic problem
- Vibrational data is scarce
- Isotopic data is lacking on many species



Status known four atom molecules (1/2)

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
c-C ₃ H	V=0	9,5, 365 GHz	None			Yes		
I-C ₃ H	nu4, Sigma	17, 360 GHz	I-C3D	nu4, Sigma	17, 360 GHz		Yes	
			13CCCH	nu4, Sigma	16, 360 GHz		Yes	
			C13CCH	nu4, Sigma	16, 360 GHz		Yes	
			CC13CH	nu4, Sigma	16, 360 GHz		Yes	
C ₃ N	nu5	30, 300 GHz	13CCCN	V=0	30, 300 GHz		Yes	
			C13CCN	V=0	30, 300 GHz		Yes	
			CC13CN	V=0	30, 300 GHz		Yes	
			CCC15N	V=0	30, 300 GHz		Yes	
C ₃ O	V=0	39, 375 GHz	None				Yes	
C ₃ S	V=0	51, 300 GHz	13CCCS	V=0	3, 17 GHz		Yes	
			C13CCS	V=0	3, 17 GHz		Yes	
			CCC34S	V=0	3, 17 GHz		Yes	
			CC13CS					
			33S, 36S					
C ₂ H ₂ *			DCCH					No rotational in HCCH
			H13CCH					Data for DCCH and DCCD at JPL
			DCCD					
NH ₃	nu2	17, 1.6 THz	H ₂ DN	V=0	20,6, 850 GHz	Yes	Yes	
			H ₃ 15N	V=0	16,16, 572 GHz	Yes		
			D ₂ HN	V=0	12,6, 515 GHz		Yes	
			D ₃ N	V=0	20,17, 612 GHz		Yes	



Status known four atom molecules (2/2)

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
HCCN	V=0	9, 198 GHz	None					
HCNH ⁺	V=0	10, 740 GHz	HCND ⁺	V=0	7, 444 GHz	Yes	Yes	
			DCNH ⁺					
			H13CNH ⁺					
			HC15NH ⁺					
HNCO	V=0	46,5, 220 GHz	None				Yes	No b-type >K=1
HNCS	V=0	85, 2, 1.07 THz	None				Yes	No b-type >K=1
HOCO ⁺	V=0	30,5, 425 GHz	None			Yes		No b-type >K=1
H2CO	V=0	45,14 2 THz	H213CO	V=0	35,10, 1.9 THz		Yes	
			HDCO	V=0	35,10, 1.6 THz		Yes	
			D2CO	V=0	40,13, 1.9 THz		Yes	
			H2C18O	V=0	30,10, 1.9 THz		Yes	
H2CN	V=0	5,4 370 GHz	None				Yes	
H2CS	V=0	26,4, 175 GHz	None				Yes	
H3O ⁺	V=0	4,3, 375 GHz	None			Yes		More data available
c-SiC3	V=0	23, 6, 275 GHz	None				Yes	



4 atom molecule work remaining

- ◆ **c-C₃H** need to be extended, 3 ¹³C isotopes need to be done, D needs to be done
- ◆ **l-C₃H** need to be extended to higher Q#, as do 3 ¹³C and D isotopes
- ◆ **C₃N** and isotopes (4) need to be extended to higher Q#, isotopes need bending state (4)
- ◆ **C₃O** need to be extended, 5 isotopes need to be done
- ◆ **C₃S** need to be extended as do 3 isotopes, 3 isotopes need to be done
- ◆ **HCCH, H¹³CCH, DCCH** need combination bands and pure rotation (>5 states)
- ◆ **¹⁵NH₃** need $\nu_2=1$ improved, **¹⁵ND_x** need to be done (3)
- ◆ **HCCN** needs to be done, very low bending need to be included, 4 isotopes are need
- ◆ **HCNH⁺, HCND⁺** need extending to 1.9 THz, 3 isotopes need to be done
- ◆ **HNCO** needs to be extended, 5 isotopes need to be done
- ◆ 6 isotopes of **HNCS** need to be done
- ◆ **HOCO⁺** need to be extended, 6 isotopes need to be done
- ◆ **H₂CN** needs to be extended, 3 isotopes need to be done
- ◆ **H₂CS** needs to be extended, 5 isotopes need to be done
- ◆ **Inversion of H₃O⁺** needs to be revisited, at least 3 isotopes need to be done
- ◆ **SiC₃** needs extending, 3 isotopes need to be done



Five atom molecules

◆ Five Atom Molecules

- Known Molecules **C₅**, C₄H, C₄Si, l-C₃H₂, c-C₃H₂, CH₂CN, CH₄, HC₃N, HC₂NC, HCOOH, H₂CNH, H₂C₂O, H₂NCN, HNC₃, **SiH₄**, H₂COH⁺
 - **Red = Not in Catalog**
- Each isotopomer and vibrational is a separate spectroscopic problem
- Vibrational data is scarce
- Isotopic data is lacking on many species



Status known five atom molecules (1/2)

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
C ₅ *	None	None	None					No dipole
C ₄ H	nu ₇ , 2nu ₇	31, 300 GHz	C ₄ D	V=0	32, 300 GHz		Yes	
			¹³ CCCCCH	V=0	30, 300 GHz		Yes	
			C ¹³ CCCH	V=0	30, 300 GHz		Yes	
			CC ¹³ CCH	V=0	30, 300 GHz		Yes	
			CCC ¹³ CH	V=0	30, 300 GHz		Yes	
C ₄ Si	V=0	48, 150 GHz	None				Yes	
I-C ₃ H ₂	V=0	18, 5, 375 GHz	I- ¹³ CCCH ₂	V=0	18, 5, 375 GHz		Yes	
			I-C ¹³ CCCH ₂	V=0	18, 5, 375 GHz		Yes	
			I-CC ¹³ CH ₂	V=0	18, 5, 375 GHz		Yes	
c-C ₃ H ₂	nu ₂ , nu ₃ , nu ₅ , nu ₆	28.23, 410 GHz	None			Yes		
H ₂ CCN	V=0	14,6, 284 GHz	None				Yes	
CH ₄ *	None	None	CDH ₃	V=0	2, 1, 280 GHz	Yes		No dipole in CH ₄ , paper in prep
			¹³C₃D					
HC ₃ N	lots	89, 810 GHz	DCCCN	nu ₇	25, 220 GHz		Yes	
			H ¹³ CCCN	5 states	70, 616 GHz		Yes	
			HC ¹³ CCN	5 states	68, 615 GHz		Yes	
			HCC ¹³ CN	5 states	68, 615 GHz		Yes	
			HCCC ¹⁵ N	5 states	69, 610 GHz		Yes	
			Doubles	V=0			Yes	



Status known five atom molecules (2/2)

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
HC ₂ NC	nu7, nu6, nu5	27, 327 GHz	None			Yes		
HCOOH	c-, t-, V=0	20,5, 295 GHz	DCOOH	V=0	30,7, 375 GHz	Yes	Yes	more data available
			H13COOH	V=0	30,9, 375 GHz	Yes	Yes	
			HCOOD	V=0	25,7, 375 GHz	Yes	Yes	
			180, 170					
H ₂ CNH	V=0	33,6, 110 GHz	H213CNH	V=0	4,1, 110 GHz	Yes		
			H2C15NH	V=0	4,1, 130 GHz	Yes		
			H2CND	V=0	13,3, 130 GHz	Yes		
			DHCNH					
			HDCNH					
H ₂ C ₂ O	V=0	39,9, 785 GHz	H213CCO	V=0	18,7, 365 GHz		Yes	
			H2C13CO	V=0	19,7, 365 GHz		Yes	
			HDCCO	V=0	26,7, 330 GHz		Yes	
			H2CC18O	V=0	20,7, 383 GHz		Yes	
			D2CCO	V=0	26,10, 340 GHz		Yes	
H2NCN	V=0	52,1, 472 GHz	None				Yes	
HNC3	V=0	5, 47 GHz	None				Yes	
SiH4*	None	None	None					No Dipole except D
H2COH+	V=0	9,3, 382 GHz	H213COH+	V=0	6,2, 220 GHz		Yes	
			D, 180					



5 atom molecule work remaining

- ◆ Vibration band of C_5 and its 5 ^{13}C isotopes are needed
- ◆ C_4H and 5 isotopes need to be extended, isotopes require low lying states (10)
- ◆ C_4Si need to be extended, 5 isotopes need to be done
- ◆ $l-C_3H_2$ and 3 isotopes need to be extended, D needs to be done
- ◆ $c-C_3H_2$ needs to be extended, 4 isotopes need to be done
- ◆ H_2CCN need to be extended, 4 isotopes need to be done
- ◆ Distortion and combination bands of CH_4 need to be done, CH_3D need to be extended, $^{13}CH_3D$ and CH_2D_2 need to be done
- ◆ $DCCCN$ needs to be extended, vibrational states of isotopes are needed (25)
- ◆ H_2CNC needs to be extended, 5 isotopes need to be done
- ◆ $HCOOH$ need to be extended and have vibrational states included, 3 isotopes need to be extended, 4 Oxygen isotopes need to be done
- ◆ H_2CNH and 3 isotopes need to be extended, 2 others need to be done
- ◆ 5 isotopes of H_2CCO need to be extended, ^{17}O needs to be done
- ◆ H_2NCN needs to be extended, 4 isotopes need to be done
- ◆ HNC_3 needs to be extended, 5 isotopes need to be done
- ◆ SiH_4 should be included, 2 isotopes should be included
- ◆ H_2COH^+ needs to be extended, 1 isotope need to be extended, 4 isotopes need to be done



Six atom molecules

◆ Six Atom Molecules

- Known molecules C_5H , $l-H_2C_4$, H_2CCH_2 , CH_3CN , CH_3NC , CH_3OH , CH_3SH , HC_3NH^+ , HC_2CHO , NH_2CHO , C_5N , $l-HC_4H$, HC_4N , $c-H_2C_3O$, H_2CCNH
 - Red = Not in catalog
- Each isotopomer and vibrational state is a separate spectroscopic problem
- Vibrational data is scarce
- Isotopic data is lacking on many species



Status known six atom molecules

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
C _s H	V=0	59, 284 GHz	C5D 13C	V=0	62, 284 GHz	Yes	Yes	
I-H ₂ C ₄	V=0	41,3, 367 GHz	I-H ₂ 13CCCC I-H ₂ C13CCC I-H ₂ CC13CC I-H ₂ CCC13C	V=0 V=0 V=0 V=0	3,1, 27 GHz 3,1, 27 GHz 3,1, 27 GHz 3,1, 27 GHz		Yes Yes Yes Yes	
C ₂ H ₄ *	None	None	None					No dipole
CH ₃ CN	nu8	85, 22, 1.4 THz	13CH ₃ CN CH ₃ 13CN CH ₃ C15N CH ₂ DCN	V=0 V=0 V=0 V=0	50, 14, 620 GHz 50, 14, 620 GHz 30, 12, 440 GHz 45, 14, 470 GHz	Yes Yes Yes Yes		perturbation not in catalog More data Koln/JPL
CH ₃ NC	V=0	7.6, 140 GHz	None			Yes		Known Poor >600 GHz
CH ₃ OH	Vt=1	20.8, 1 THz	13CH ₃ OH CH ₂ DOH CH ₃ 18OH CH ₃ OD CD ₂ HOH CD ₃ OH 17O, 13C&Ds	Vt=1	20.8, 1 THz		Yes	Known line strength prolem JPL has data Data available Data available Some OSU data Data available No data
CH ₃ SH	None	None	None					Data available
HC ₃ NH.	V=0	4, 36 GHz	None				Yes	
HC ₂ CHO	V=0	23,14, 188 GHz	None			Yes		
NH ₂ CHO	V=0	4.2, 84 GHz	None			Yes		
C ₅ N	V=0	6, 17 GHz	None				Yes	
I-HC ₄ H*	None	None	None					No dipole
I-HC ₄ N	V=0	7, 33 GHz	None			Yes		
c-H ₂ C ₃ O	V=0	24,12, 250 GHz	None				Yes	
H ₂ CCNH	V=0	Low J, freq	None				Yes	



6 atom molecule work remaining

- ◆ 5 ^{13}C isotopes of C_5H need to be done, bending modes (3) of C_5H are needed
- ◆ l- H_2CCCC needs to be extended as do 4 isotopes DHCCCC needs to be done
- ◆ HDCCH₂ needs to be done, H_4C_2 and ^{13}C needs to be checked for distortion allowed and combination bands
- ◆ CH_3CN need to include more vibrational states, perturbation with nu8, 4 isotopes need extending and nu8, doubles (6) need to be done
- ◆ CH_3NC needs to be extended, 4 isotopes need to be done
- ◆ CH_3OH needs to be extended to $J=45+$, $v_t=2,3,4$ V_{OH} need to be included as do torsional transitions, ^{13}C needs extended, all combinations of isotopes are needed, singles should include $vt=1$ at least, dipole needs to be fixed
- ◆ CH_3SH needs to be done, 6 isotopes need to be done
- ◆ HC_3NH^+ needs to be extended, 6 isotopes need to be done
- ◆ HC_2CHO needs to be extended, 7 isotopes need to be done
- ◆ NH_2CHO needs to be extended, 6 isotopes need to be done
- ◆ C_5N needs to be extended, 6 isotopes need to be done
- ◆ Vibrational band of l- HC_4H needs to be included, as to 5 isotopes
- ◆ l- HC_4N needs to be extended, 6 isotopes need to be done
- ◆ c- $\text{H}_2\text{C}_3\text{O}$ need to be extended, 6 isotopes need to be done
- ◆ H_2CCNH needs to be extended, 5 isotopes need to be done



Seven atom molecules

◆ Seven Atom Molecules

- Known molecules C_6H , CH_2CHCN , CH_3CCH , HC_5N , CH_3CHO , CH_3NH_2 , $c-C_2H_4O$, H_2CCHOH
 - Red = Not in catalog
- Each isotopomer and vibrational state is a separate spectroscopic problem
- Vibrational data is scarce
- Isotopic data is lacking on many species



Status known seven atom molecules

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS		
C ₆ H	V=0	79, 220 GHz	13CC5H	V=0	8, 21 GHz	Yes	Yes		
			C13CC4H	V=0	8, 21 GHz		Yes		
			C213CC3H	V=0	8, 21 GHz		Yes		
			C313CC2H	V=0	8, 21 GHz		Yes		
			C413CCH	V=0	8, 21 GHz		Yes		
			C513CH	V=0	8, 21 GHz		Yes		
			C6D	V=0	60, 158 GHz			Yes	
CH ₂ CHCN	V=0	26,17, 210 GHz	CH2CH13CN	V=0	3,2, 30 GHz	Yes			
			CH213CHCN	V=0	3,2, 30 GHz	Yes			
			13CH2CHCN	V=0	3,2, 30 GHz	Yes			
			CH2CDCN	V=0	3,2, 30 GHz	Yes			
			15N, D _{x2}						
CH ₃ C ₂ H	nu10, nu9	55,14, 920 GHz	CH3C2D	V=0	29,18, 451 GHz		Yes		
			CH2DC2H	V=0	33,12, 467 GHz		Yes		
			13C						
HC ₅ N	v11=0-4, v9, v7	182, 457 GHz	DC5N	V=0	190, 456 GHz		Yes		
			H13CC4N	V=0	73,189 GHz		Yes		
			HC13CC3N	V=0	71, 187 GHz		Yes		
			HC213C2N	V=0	71,188 GHz		Yes		
			HC313CCN	V=0	71,188 GHz		Yes		
			HC413CN	V=0	72, 190 GHz		Yes		
			HC515N	V=0	72, 187 GHz		Yes		
CH3CHO	V=0	12,3, 120 GHz	None					Data available, more at JPL	
CH3NH2	None	None	None						Data available
c-C ₂ H ₄ O	V=0	50,30, 357 GHz	None						
H ₂ CCHOH	s-, a-	25,5, 110 GHz	None						



7 atom molecule work remaining

- ◆ 5 ^{13}C isotopes of C_5H need to be extended
- ◆ CH_2CHCN need to be extended as do 4 isotopes, 3 isotopes need to be done, 3 low lying vibrational states are need
- ◆ 2 isotopes of CH_3CCH need to be extended, 3 ^{13}C isotopes need to be done
- ◆ CH_3CHO need to be extended to $J=50$, $vt=2$, 6 isotopes need to be done, low lying vibration is also needed.
- ◆ CH_3NH_2 need to be included, 4 isotopes need to be done. Low lying torsion and inversion need to be done. New physics is involved
- ◆ 8 isotopes of $\text{c-C}_2\text{H}_4\text{O}$ need to be done
- ◆ H_2CCHOH need to be extended, 8 isotopes need to be done



8 atom molecules

◆ Eight Atom Molecules

- Known Molecules $\text{CH}_3\text{C}_3\text{N}$, HCOOCH_3 , CH_3COOH , C_7H , H_2C_6 , CH_2OHCHO , $\text{I-HC}_6\text{H}$, CH_2CHCHO , CH_2CCHNC
 - Red = Not in Catalog
- No isotopic data
- No vibrational data



Status known eight atom molecules

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
CH ₃ C ₃ N	V=0	70,15, 290 GHz	None				Yes	
HCOOCH ₃	V=0	50,30, 550 GHz	None			Yes		More data available
CH ₃ COOH	None	None	None					
C ₇ H	V=0	122, 195 GHz	None				Yes	
H ₂ C ₆	V=0	7.1, 18 GHz	None				Yes	
CH ₂ OHCHO	V=0	55,25, 355 GHz	None				Yes	
I-HC ₆ H*	None	None	None					No dipole
CH ₂ CHCHO	V=0	20,18, 179 GHz	None			Yes		
CH ₂ CCHCN	V=0	34,20, 179 GHz	None				Yes	



8 atom molecule work remaining

- ◆ $\text{CH}_3\text{C}_3\text{N}$ need to include low lying vibration, 6 isotopes need to be done
- ◆ HCOOCH_3 (methyl formate) needs to include $\nu_t=1$, 8 isotopes need to be done
- ◆ CH_3COOH (Vinegar) need to be included and extended to $\nu_t=3$, 8 isotopes need to be done
- ◆ 8 isotopes of C_7H need to be done
- ◆ H_2C_6 needs to be extended, 7 isotopes need to be done
- ◆ CH_2OHCHO needs to include low lying vibrational states 10 isotopes need to be done
- ◆ Bending mode of $\text{l-HC}_6\text{H}$ needs to be done, as do 7 isotopes
- ◆ CH_2CHCHO need to be extended, low lying vibrational states need to be done, 9 isotopes need to be done
- ◆ CH_2CCHCN needs to be extended, low lying vibration states need to be done, 8 isotopes need to be done



9 atom molecules

◆ Nine Atom Molecules

- Known Molecules $\text{CH}_3\text{C}_4\text{H}$, $\text{CH}_3\text{CH}_2\text{CN}$, $(\text{CH}_3)_2\text{O}$, $\text{CH}_3\text{CH}_2\text{OH}$, HC_7N , C_8H , $\text{CH}_3\text{C}(\text{O})\text{NH}_2$
 - Red = Not in Catalog
- Only one (HC_7N) with any vibrational data
- Minimal isotope data
- Very thin coverage



Status known nine atom molecules

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
CH3C4H	V=0	55,15, 224 GHz	None				Yes	
CH3CH2CN	V=0	65,36, 610 GHz	13CH3CH2CH	V=0	5,3, 55 GHz	Yes		vt=1, out of plane bend at JPL
			CH313CH2CN	V=0	5,3, 55 GHz	Yes		
			CH3CH213CN	V=0	5,3, 55 GHz	Yes		
			CH3CH2C15N	V=0	5,3, 55 GHz	Yes		
			CH2DCH2CN	V=0	5,3, 55 GHz	Yes		
(CH3)2O	V=0	23,5, 224 GHz	None			Yes		Data available, more at Koln/JPL
CH3CH2OH	V=0	30,10, 500 GHz	None			Yes		JPL data to 1.6 THz
HC7N	nu15=0-2	211, 225 GHz	DC7N	V=0	13, 15 GHz	Yes		
			H13CC6N	V=0	13, 15 GHz	Yes		
			HC13CC5N	V=0	13, 15 GHz	Yes		
			HC213CC4N	V=0	13, 15 GHz	Yes		
			HC313CC3N	V=0	13, 15 GHz	Yes		
			HC413CC2N	V=0	13, 15 GHz	Yes		
			HC513CCN	V=0	13, 15 GHz	Yes		
			HC613CN	V=0	13, 15 GHz	Yes		
			HC715N	V=0	13, 15 GHz	Yes		
C8H	V=0	85, 99 GHz	None					
CH3C(O)NH2	None	None	None					



9 atom molecule work remaining

- ◆ $\text{CH}_3\text{C}_4\text{H}$ low lying vibrations are needed, 7 isotopes are needed
- ◆ $\text{CH}_3\text{CH}_2\text{CN}$ requires 6 vibrational states, 5 isotopes require extending, 2 require doing (vibrational states are new physics)
- ◆ $(\text{CH}_3)_2\text{O}$ requires extending and both $\nu_t=1$ states, 4 isotopes (D is new physics)
- ◆ $\text{CH}_3\text{CH}_2\text{OH}$ requires extending, $\nu_{\text{OH}}=1$, $\nu_{\text{CH}_3}=1$, 8 isotopes (torsion is new physics)
- ◆ 9 isotopes of HC_7N need extending
- ◆ 9 isotopes of C_8H need to be done
- ◆ $\text{CH}_3\text{C}(\text{O})\text{NH}_2$ need to be done, 8 isotopes need to be done



Ten and Large atom molecules

◆ Ten Atom Molecules

- Known Molecules $\text{CH}_3\text{C}_5\text{N}$, $(\text{CH}_3)_2\text{CO}$, $(\text{CH}_2\text{OH})_2$, $\text{H}_2\text{NCH}_2\text{COOH}$, $\text{CH}_3\text{CH}_2\text{CHO}$
 - Red = Not in Catalog
- No vibrational data
- No isotopic data

◆ Eleven & Large Atom Molecules

- Known Molecules HC_9N , C_6H_6 , $\text{C}_2\text{H}_5\text{OCH}_3$, HC_{11}N
 - Red = Not in Catalog
- No vibrational data
- No isotopic data



Status known 10+ atom molecules

Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
CH3C5N	V=0	25.6, 40 GHz	None				Yes	
(CH3)2CO	None	None	None					Data on vt=1 available
(CH2OH)2	aGg', gGg'	50,20, 350 GHz	None				Yes	
CH3CH2CHO	None	None	None					
11 atoms								
Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
HC9N	V=0	18, 11 GHz	None			Yes		
CH3C6H	V=0	25,9, 40 GHz	None				Yes	
12 atoms								
Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
C6H6*	None	None	None					No Dipole
C2H5OCH3	None	None	None					
13 atoms								
Molecule	V's	N,K Freq	Isotopes	V's	N,K Freq	JPL	CDMS	
HC11N	V=0	43, 15 GHz	None			Yes		



10+ atom molecule work remaining

- ◆ $\text{CH}_3\text{C}_5\text{N}$ need to be extended, 8 isotopes need to be done, low lying bending modes are needed (>3)
- ◆ $(\text{CH}_3)_2\text{CO}$ need to be included, 5 isotopes need to be done (D is new physics), at least the lowest two torsional states are needed
- ◆ $\text{CH}_3\text{CH}_2\text{CHO}$ need to be included and extended to higher frequencies, 9 isotopes need to be done, low lying vibrations (>3) and torsion should be done
- ◆ HC_9N needs to be extended, 11 isotopes need to be done, low lying bending band is needed
- ◆ $\text{CH}_3\text{C}_6\text{H}$ need to be extended, 9 isotopes need to be done, lowest bending band is needed
- ◆ IR puckering band of C_6H_6 should be included
- ◆ $\text{C}_2\text{H}_5\text{OCH}_3$ needs to be included, 9 isotopes need to be measured, lowest torsion and vibration need to be measured



What has not been considered

- ◆ **Lines of “expected species”**
 - **Chemical models require many molecules to work**
 - E.g. NH^+ , NH_2^+ , NH_3^+ , NH_4^+ , NH , CH_2^+ , CH_3 , CH_3^+ , CH_5^+ , OH^- , OH^+ ,
 - **Metal hydrides and oxides likely in late type stars and shells**
 - **PAH molecules**

- ◆ **Little data on potential larger molecules in the 480+ GHz range!**

- ◆ **Less data on vibrational and torsional transitions**

- ◆ **Majority of problems require spectroscopy before it is possible to catalog**
 - **Only a handful have high quality data available**



Summary

- ◆ **60 diatomic molecules need to be measured or have additional measurements**
- ◆ **120 triatomic molecules need to be measured or have additional measurements**
- ◆ **100 4 atom molecules need to be measured or have additional measurements**
- ◆ **130 5 atom molecules need to be measured or have additional measurements**
- ◆ **130 6 atom molecules need to be measured or have additional measurements**
- ◆ **60 7 atom molecules need to be measured or have additional measurements**
- ◆ **95 8 atom molecules need to be measured or have additional measurements**
- ◆ **70 9 atom molecules need to be measured or have additional measurements**
- ◆ **70 10+ atom molecules need to be measured or have additional measurements**
- ◆ **Total is 835 pieces of spectroscopy and/or cataloging are need**
 - **Priorities should be considered carefully**