Herschel Spectroscopic Lessons for ALMA

John C. Pearson
Jet Propulsion Laboratory, California Institute of Technology

Abstract:

Spectroscopy with Herschel provides a unique opportunity to determine what might be expected from ALMA. Herschel's Heterodyne Instrument for Far Infrared (HIFI) has a specifically designed line survey mode, which allows for comprehensive spectroscopy, providing enormous insight into what is present in the gas phase. HIFI data coupled with ground based interferometer observations quickly show that the typical rich molecular source size is much smaller than the beam of the 3.5 meter Herschel telescope. As such, the observed HIFI spectra is usually a convolution of several sources within the beam. Regardless, HIFI has shown rich line sources to be very bright to well over 1 THz or the entire ALMA band. ALMA will fully resolve many sources even in its most compact configuration so that the only dilution will be the aperture filling factor. The HIFI observations, estimated source sizes and ALMA sensitivities allow for calculation of what to expect in ALMA data. In the absence of line confusion, ALMA can be expected to produce spectra with similar dynamic range to the best available laboratory spectra. These expectations are compared to available molecular data for Methanol and Ethyl Cyanide to provide an example of what will be required from catalogs, laboratory astrophysicist and astrophysical spectroscopists in the ALMA era.

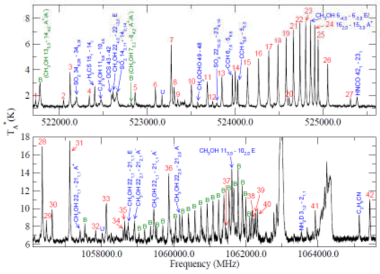
Anatomy of Hot Dense Cores:

Internal heating from (forming) internal central star: Compression heating, UV field, Bipolar Outflows, Shocks. Results in small hot region surrounded by progressively cooler gas. Typically modeled with two or more components one small, hot, and usually optically thick on strong lines the others are progressively larger and cooler with less opacity.

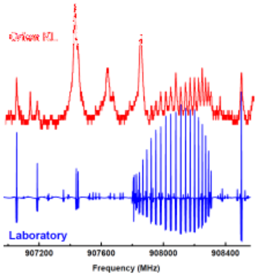
External heating from gas swept up by radiation pressure from O & B-stars: Compression heating, UV field, Shocks. Results in a small hot edge region flanked on one side with progressively cooler gas. Typically modeled with two or more components one small hot and often optically thick on strong lines the other components are progressively larger and cooler with less opacity.

The hot dense components are generally small compared to the HIFI beam and have derived temperatures of ~200K while the colder components can fully fill the beam in more local cases.

Orion KL from HIFI HEXOS Observations



Spectra of Orion KL showing the ground J_{-4} to J_{-3} E state Q-branch (top) $J_{max}=34$ and the ground J_7 to J_6 A state Q-branch (bottom) most of this branch has unresolved asymmetry splitting. Many other methanol lines are observed ($J_{K,vt}$ is labeled) or numbered. From Wang et al. 2011.

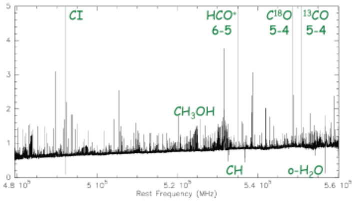


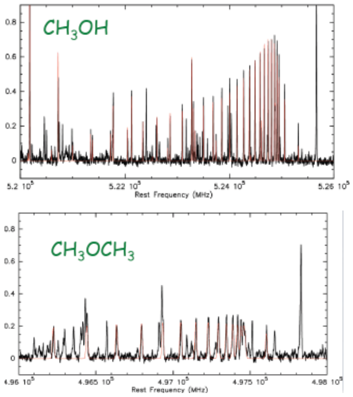
Orion KL spectra near 908 GHz compared to laboratory spectrum of methanol. The $v_t=2$ J_4 to J_3 A state Q branch, $J_{max}=19$. Branch origin is on the right at 638 K above ground. Asymmetry splitting becomes apparent before the turning point on the right.

HIFI clearly sees the hot gas even though we believe that observations are significantly beam diluted. ALMA will resolve the small hot region. This will facilitate observation of higher J observations and more excited vibrational and torsional states.

The current sensitivity driven limits for methanol laboratory data are J~45 in $v_t=0$, J~43 in $v_t=1$, J~41 in $v_t=2$ and J~33 in $v_t=3$. Hamiltonian modeling has only considered J=30 and $v_t=0,1,2$. Some microwave transitions of $v_t=4$, $\nu_8=1$ and $\nu_7=1$ have also been identified but there have been only been comprehensive infrared studies.

NGC6334I from HIFI CHESS Observations





NGC6334I similar to Orion KL but further away and in a slightly different state of chemical evolution. Lots of hot complex molecules.

The ALMA Challenge for Methanol

Assuming a hot region of 2 arcsec in size a 200K excitation temperature with ΔT=160K of gas-dust temperature and the strongest methanol lines having opacities of τ=10, the peak line strengths of the methanol bands would be as follows

$v_t=1$ @ 207.4 cm^{-1}	Optically thick τ=4
$v_t=2$ @ 353.2 cm^{-1}	125 K
$v_t=3$ @ 670.5 cm^{-1}	13 K
$v_t=4$ @ 1046.9 cm^{-1}	850 mK
$v_t=5$ @ 1651.8 cm^{-1}	11 mK
ν_8 (CO stretch) @ 1033.5 cm^{-1}	944 mK
ν_7 (CH_3 rock in-plane) @ 1074.5 cm^{-1}	703 mK
ν_{11} (CH_3 rock out-of plane) @ 1145 cm^{-1}	423 mK
ν_6 (OH bend) @ 1339.5 cm^{-1}	104 mK
ν_5 (CH_3 symmetric bend) @ 1454.5 cm^{-1}	46 mK
ν_{10} (CH_3 asymmetric bend) @ 1465 cm^{-1}	42 mK
ν_4 (CH_3 asymmetric bend) @ 1478.4 cm^{-1}	38 mK

Using the ALMA sensitivity calculator for 50 Antennas, ALMA will reach 76 mK in a 2 arcsec beam in a 1 MHz bandwidth in 1 minute at 310 GHz and 87 mK in for the same conditions at 640 GHz. Assuming the ALMA stability is sufficient to integrate as the square root of time a deep 400 minute integration would achieve ~4 mK RMS and detect all of these band! Even in 1 minute $v_t=4$ and the three lowest vibrational states are easily detected! A one minute integration is comparable to a good laboratory spectrum. A deep integration is as good or better than the best available laboratory spectrum.

Assuming H/D of 6000, $^{12}C/^{13}C$ of 50 and $^{16}O/^{17}O$ of 2500 $^{16}O/^{18}O$ of 500:
$^{13}CH_3OH$ ground state is 32K states through $v_t=3$ are seen in 1 minute
$CH_3{}^{18}OH$ ground state is 3.2K states though $v_t=2$ are seen in 1 minute
CH_2DOH ground state is 800mK $v_t=1$ is seen in 1 minute
$CH_3{}^{17}OH$ ground state is 640mK $v_t=1$ is seen in 1 minute
$^{13}CH_3{}^{18}OH$ ground state is 64mK

Microwave spectroscopy of $v_t=0,1,2$ &3 is done. IR spectroscopy of $v_t=4$, ν_8, most of ν_7 and ν_{11} is done but microwave spectrum remains to be measured. Higher in energy methanol is less well described. Physics required for analysis and accurate calculation of intensities must be developed for the vibrational states of methanol. Significant expansion of data for several isotologues is also going to be necessary.

The ALMA Challenge for CH_3CH_2CN

Assuming a hot region of 2 arcsec in size a 200K excitation temperature with ΔT=160 K of gas-dust temperature and the strongest ground state CH_3CH_2CN lines being 40 K, the line strengths of CH_3CH_2CN bands would be as follows:

ν_{13} (in-plane CCN bend)*	206.9 cm^{-1}	9 K
ν_{21} (CH_3 torsion, $v_t=1$)*	213.1 cm^{-1}	8.6 K
ν_{20} (out-of-plane CCN bend)*	370.3 cm^{-1}	2.8 K
$2\nu_{13}$ (in-plane CCN overtone)	411cm^{-1}	2.1 K
$2\nu_{21}$ ($v_t=2$)	412 cm^{-1}	2.1 K
$\nu_{13}+\nu_{21}$ ($v_t=1$ of ν_{13})	417 cm^{-1}	2 K
ν_{12} (CCC bend)*	534.4 cm^{-1}	860 mK
$\nu_{20}+\nu_{13}$ (CCN in and out of plane combination)	577 cm^{-1}	630 mK
$\nu_{20}+\nu_{21}$ ($v_t=1$ of CCN out of plane bend)	583 cm^{-1}	600 mK
$3\nu_{21}$ ($v_t=3$)	625 cm^{-1}	445 mK
$3\nu_{13}$ (in-plane CCN 2nd overtone)	618 cm^{-1}	465 mK
$\nu_{13}+2\nu_{21}$ ($v_t=2$ of in-plane CCN bend)	625 cm^{-1}	445 mK
$2\nu_{13}+\nu_{21}$ ($v_t=1$ of CCN overtone)	630 cm^{-1}	430 mK
ν_{19} (CH_3 rock out of plane)	784.5 cm-1	140mK
ν_{11} (CH_3 rock in plane)	836.5 cm-1	97mK

States below 1150 cm^{-1} will be greater than 10 mK. 45% of population is in excited vibrational states.
*Previously detected

Physics remains to be worked out for everything above ν_{21}. Isotopologues are also a problem Single ^{13}C is 800mK (three of them) lowest 2 states ~180 mK, $^{14}N/^{15}N=250$ ^{15}N is 160 mK double ^{13}C is 16 mK. Lots will be seen instantly with ALMA. Data bases for weeds still need enormous improvements.

References on Methanol:
L.-H. Xu, J. Fisher, R.M. Lees, H.Y. Shi, J.T. Hougen, J.C. Pearson, B.J. Drouin, G.A. Blake & R. Braakman, 2008, J. Mol. Spectrosc. 251, 305.
J.C. Pearson, C.S. Brauer, B.J. Drouin & L.-H. Xu, 2009, Can. J. Phys. 87, 449.
S. Wang, et al., 2011, A&A in press.
References on CH_3CH_2CN:
H.M. Heise, F. Winther & H. Lutz, 1981, J. Mol. Spectrosc. 90, 531.
D.M. Meringer, J.C. Pearson, J. Keene & T.G. Phillips, 2004, ApJ 608, 306.
C.S. Brauer, J.C. Pearson, B.J. Drouin & S. Yu, 2009, ApJS184, 133.

Acknowledgement: This research was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contract with the National Aeronautics and Space Administration. Funding from the NHSC and APRA are also greatfully acknowledged.

National Aeronautics and Space Administration

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

www.nasa.gov