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- Molecular lines
- Science overview
- Toward the future

At 100 GHz ($\lambda = 3$ mm): E = hv/q = 4 x 10⁻⁴ eV T = hv/k = 5 K

This tells us what kind of phenomena we will be dealing with.

But first, a few words about the earth's atmosphere...





The distance from here to the stratosphere is roughly the same as the distance from Epping to the Sydney Opera House.

















 RAR, Pacea de Brer, France
 pagea de la manufactura



BIMA—the Berkeley/Illinois/Maryland Array, Hat Creek, California.

http://bi



Owens Valley Radio Observatory, California



The mm upgrade and operation of Mopra Observatory is a collaboration between UNSW and ATNF.



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The bigger the molecule, the larger the *partition function*.

That is to say, at any given temperature the molecules can be distributed over a larger number of available energy levels.

For any given molecule, increasing the temperature will increase the population in higher lying states, while decreasing that in the lower.

V	2					
950 -	1		14			
900-	-30cm ¹			20		
850 -				25		54
000						
750-	-25cm			-23		50
700-	3					-49
650-				<u></u> n		47
600-	-20cm ¹					
-						
300-		3				-43
500-			10			
450-	-15cm ¹					
400-	MBER		9			
350 -	R2				-25	
300-	Demi		8	15	23	33
250		<u> </u>	-7		-22	=3
2.30				13		
200-			6	-11	-18	<u>_</u> 28
150 -	-5cm ¹		5			=
100 -	1	1			≡ ₿	=
50-		_	-3	7	≡ ₩	15
			2	=3.		10
0-	J=0	HCN J=0	HC ₂ N ^{J=0}	HC _s N J=0	HC7N J=0	HC ₉ N J=0

Line Intensities (linear molecules)

Only certain transitions are permitted.

For dipole-allowed transitions they are those with $\Delta J = \pm 1$.

We have $A_{ij} \alpha \upsilon^3 |\mu_{ij}|^2$,

Where A_{ij} is the *dipole moment matrix element* connecting the two states i and j, and depends on the molecule's dipole moment, μ .

For CO, $\mu = 0.10$ D. For HCN, $\mu = 3.00$ D.

Line Intensities (linear molecules)

For CO, $\mu = 0.10$ D. For HCN, $\mu = 3.00$ D.

The A coefficient for the $J = 1 \rightarrow 0$ transition of HCN is therefore ~1000 times that of CO.

Molecules such as N_2 and H_2 have no dipole moment and thus have no dipole-allowed transitions.

Line Intensities (any molecule)

The observed emission line intensity depends on the A coefficient, A_{ij} , and the column density of molecules in the upper state, which in turn depends on:

- The column density of H_2
- The molecular abundance relative to H₂
- The molecular partition function
- The temperature of the gas
- The density of the gas.

(Assuming, of course, that the line is *optically thin*. If it is *optically thick*, the intensity depends **only** on the gas temperature.)



We then set up a Hamiltonian

 $H = AP_{a}^{2} + BP_{b}^{2} + CP_{c}^{2}$,

where P_a etc is the component of angular momentum along that axis.

We then solve Schrödinger's equation to obtain the energy levels.

If A = B = C, we have a *spherical top*, which is unlikely to be interesting (eg, methane).

If A > B = C, we have *prolate* (ie, cigar shaped) *symmetric top* (eg methyl cyanide).

If A = B > C, we have an *oblate* (ie pancake shaped) *symmetric top* (eg ammonia).

If A > B > C, we have an *asymmetric top* (eg water) and a very complicated spectrum.

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The energy levels of a prolate symmetric top are given by $E_{JK} = BJ(J+1) + (A-B)K^2$

and for an oblate symmetric top by $E_{JK} = BJ(J+1) + (C\mbox{-}B)K^2 \label{eq:element}$

where K is the component of angular momentum along the symmetry axis of the molecule.

Note that ΔE does not depend on K to first order; however it does when centrifugal distortion is taken into account.



K is the projection of the total angular momentum on the symmetry axis.

For a symmetric top, the dipole-allowed transitions are those with $\Delta J = 0, \pm 1$ and $\Delta K = 0.$

From Gordy and Cook (197













Asymmetric tops

The three rotational constants (A, B & C) are all different.

Each energy level is characterised by three quantum numbers: J, $K_{\text{-}1}$, $K_{\text{+}1}.$

In the worst-case scenario, we will have 3 dipole moment components (μ_A , μ_B , μ_C) and lines all over the place.

While we *could* calculate their frequencies, we will more likely just look them up at:

up at: http://physics.nist.gov/PhysRefData/micro/html/contents.html



Nuclear quadrupole splitting.

If a molecule contains a nucleus with a nuclear spin, I, of 1 or more, the interaction between the nuclear quadrupole moment and the molecular electric field gradient results in splitting of the energy levels.

Single lines become *multiplets*.

From Gordy and Cook (1970)

¹⁴N has I = 1, and hence N-containing molecules exhibit quadrupole splitting.



Non-comformist molecules.

• OH has an unpaired electron and a ${}^{2}\Pi$ ground state, leading to *A-doublet* transitions at cm wavelengths.

• O₂ is symmetrical like N₂, but has a ${}^{3}\Sigma$ electronic ground state (instead of ${}^{1}\Sigma$), leading to *magnetic dipole-allowed* transitions.

• NH₃ can undergo an *inversion* motion, like an umbrella on a windy day, leading to transitions throughout the 12 mm region.





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Science

- Atmospheric science
- Planetary science
- Star formation
- Post AGB stars and planetary nebulae
- AGNs, Galaxy evolution and cosmology
- Cosmic microwave background



Mm observations provide data on trace atmospheric gasses important to ozone depletion and global warming studies.

http://seds.lpl.arizona.ed



http://cfa-

• resolve planetary disks to study variation of

atmosphere with position and time • study atmospheric dynamics through direct

observation of doppler shifts in line cores









Galaxy Evolution and Cosmology arcsec efi: 850µm SCUBA image of the Hubble Deep Field showing a new population of dusty gain. Right: Lensed CO J=?-6 emission from the Cloverlanf queen imaged by the BEAM PdBL http:/ /cfa-www.harvard.edu/~dw





http://maisel.as.arizona.edu:8080/bitmaps/COBE.jpg

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ALMA



The Atacama Large MM Array



Proposed: 64 6-metre dishes; up to 10 km baseline.





References

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