

Practical work on Spectroscopy: Identifying molecules in spectra

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When dealing with observed spectra containing molecular lines the first step we have to take is the identification of the lines. If the spectrum displays lines of well characterized molecules from the spectroscopically point of view the identification is usually relatively easy provided the signal-to-noise ratio of the lines sufficiently high. Otherwise, the effect of noise can make this task more complex. Under favorable conditions the identification process can be completed in a more or less short time taking advantage of public or private databases.

Nevertheless, the line identification process is not that easy when we have the spectra of unknown molecules. Not all the molecules are spectroscopically well characterized commonly due to their properties, which can favor fast condensation into solid state in refractory molecules, or serious difficulties during the experimental synthesis of the species. Despite the very important output of numerical methods, their descriptions of the energy levels are most of the times not good enough to produce accurate data that can be directly compared with observations without an experimental guidance.

There is not a well defined method to identify the carriers of these unknown molecules in a general case but for simple molecules the procedure is much better constrained. This method is based on determining the rotational constants from the observed spectrum and comparing them with tabulated values. How you get to these values is another matter that we will not address here and can involve very sophisticated techniques.

Goals

The spectrum to be studied is shown in the Figure of the next slide and the data is provided in an ascii file composed of only two columns: frequency in MHz and main beam temperature (T_{mb}) in K. Note that the average frequency of the spectrum is $\simeq 40$ GHz, typical of the Q branch which is covered by the Yebes RT40m telescope, operated by the Observatorio Astronómico Nacional (OAN). These frequencies imply that *the spectrum only comprises pure rotational lines*. In this particular case, molecules are vibrating in the ground state ($v = 0$) and the electronic state is also the ground.

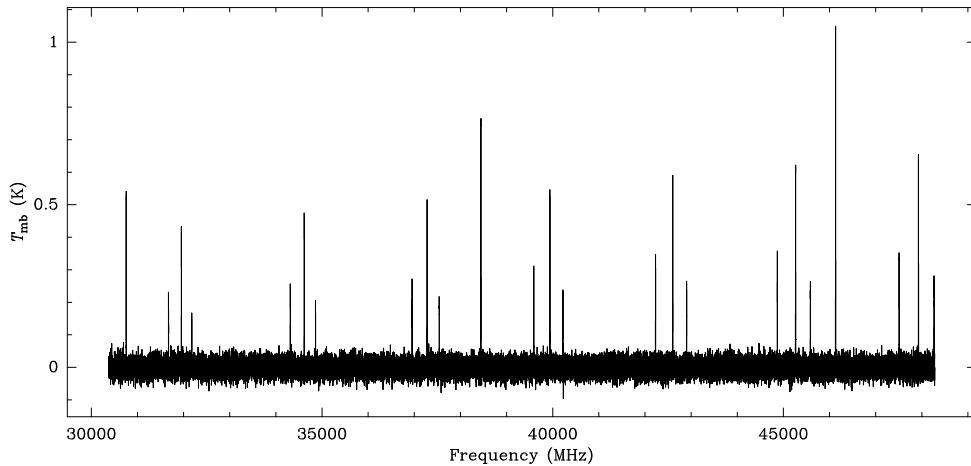
The goals of this practical work are:

- To identify what lines belong to each spectrum,
- To extract the rotational constant(s) corresponding to at least one molecule, and
- To compare these constant(s) with those included in the Table in the next slide to figure out what molecules are producing the observed lines.

RECOMMENDATION

Start always from the simplest case

Data: <https://saco.csic.es/s/x5DS4N34MtBQcjm>



Molecule	A (MHz)	B (MHz)	C (MHz)	Molecule	A (MHz)	B (MHz)	C (MHz)
HCN	—	44315.976	—	K ³⁵ Cl	—	3850.4495	—
CO	—	57635.968	—	c-C ₃ H ₂	35092.51	32212.95	16749.03
HC ₃ N	—	4549.059	—	HCNO	—	11469.05	—
HC ₅ N	—	1331.3327	—	t-HCOOH	77512.24	12055.021	10416.200
SiO	—	21711.9675	—	HCCP	—	5623.116	—
AlF	—	16488.355	—	HMgC ₃ N	—	1319.72	—
PH ₃	133480.128	133480.128	117489.43	H ₂ C ₄ O	~282000	2160.72	2146.84
AlC ₃ N	—	1340.758	—	HOCHCHCHO	9839.956	5185.627	3393.807

Top type	Top subtype	Quantum numbers	Condition	E_{rot}
Linear (+diatomic)	—	J	$A = C = 0, B \neq 0$	$BJ(J+1)$
Spherical	—	J	$A = B = C$	$BJ(J+1)$
Symmetric	Prolate	J, K	$A > B = C$	$BJ(J+1) + (A-B)K^2$
Symmetric	Oblate	J, K	$A = B > C$	$BJ(J+1) - (B-C)K^2$
Asymmetric	—	J, K_a, K_c	$A > B > C$	$BJ(J+1) + (A-B)K_a^2 - (B-C)K_c^2$

$$\nu = E_{\text{up}} - E_{\text{low}} \quad , \quad \Delta J = 1$$