Status and prospects of molecular buffer gas cooling

KITP discussion, 4/20/18

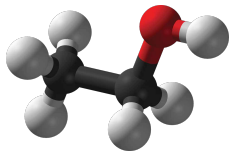
davepatterson@ucsb.edu
http://pattersongroup.physics.ucsb.edu

We can make lots of molecules pretty cold

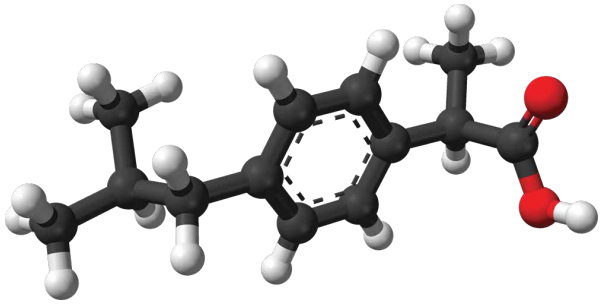
$N \approx 10^{14}$ at a time

$T \approx 5$ K

"Any molecule"

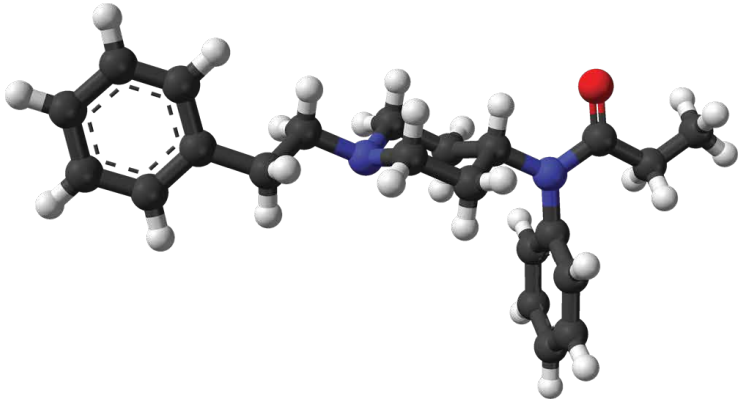


Is this good for anything?

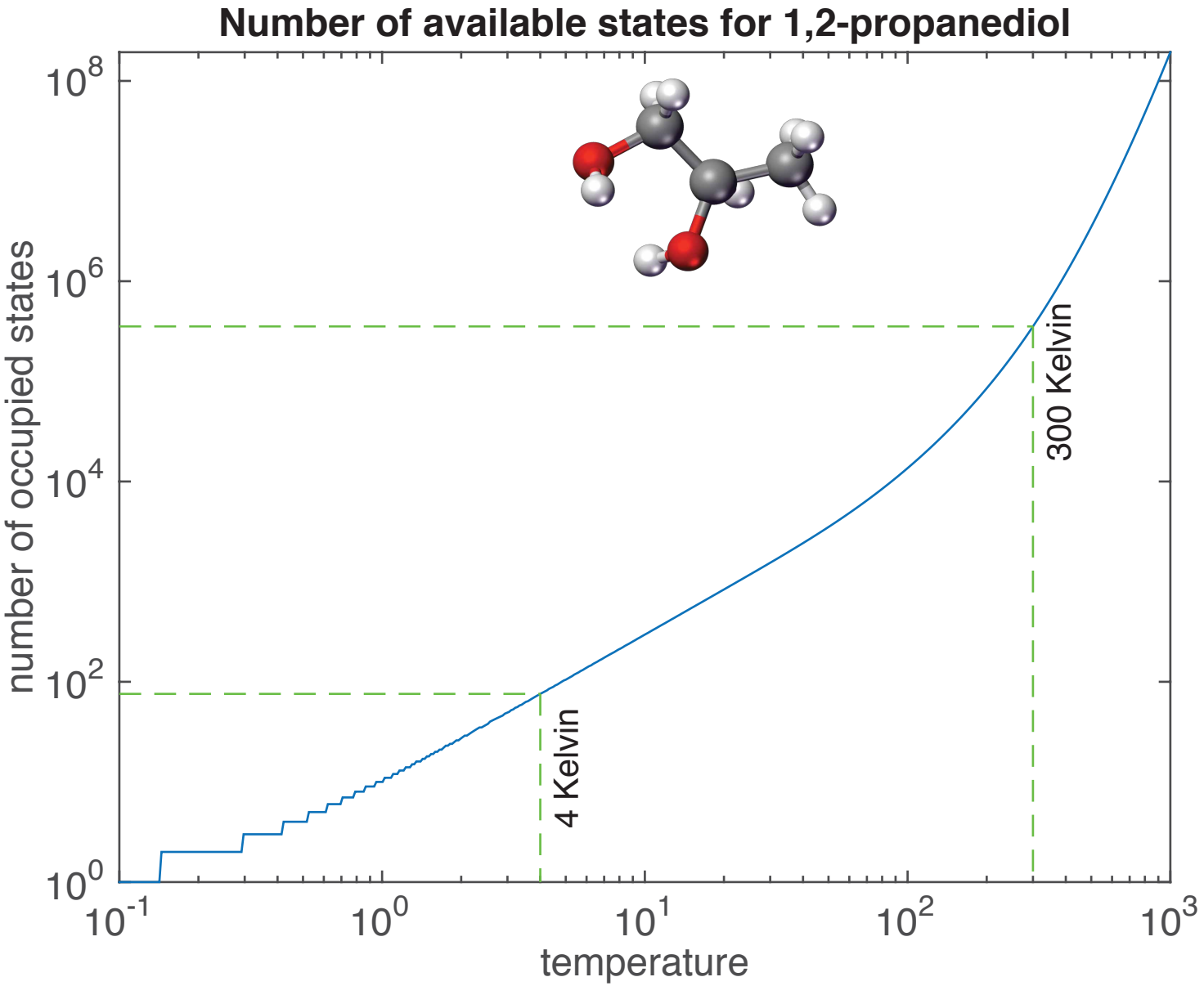


-BSM physics?

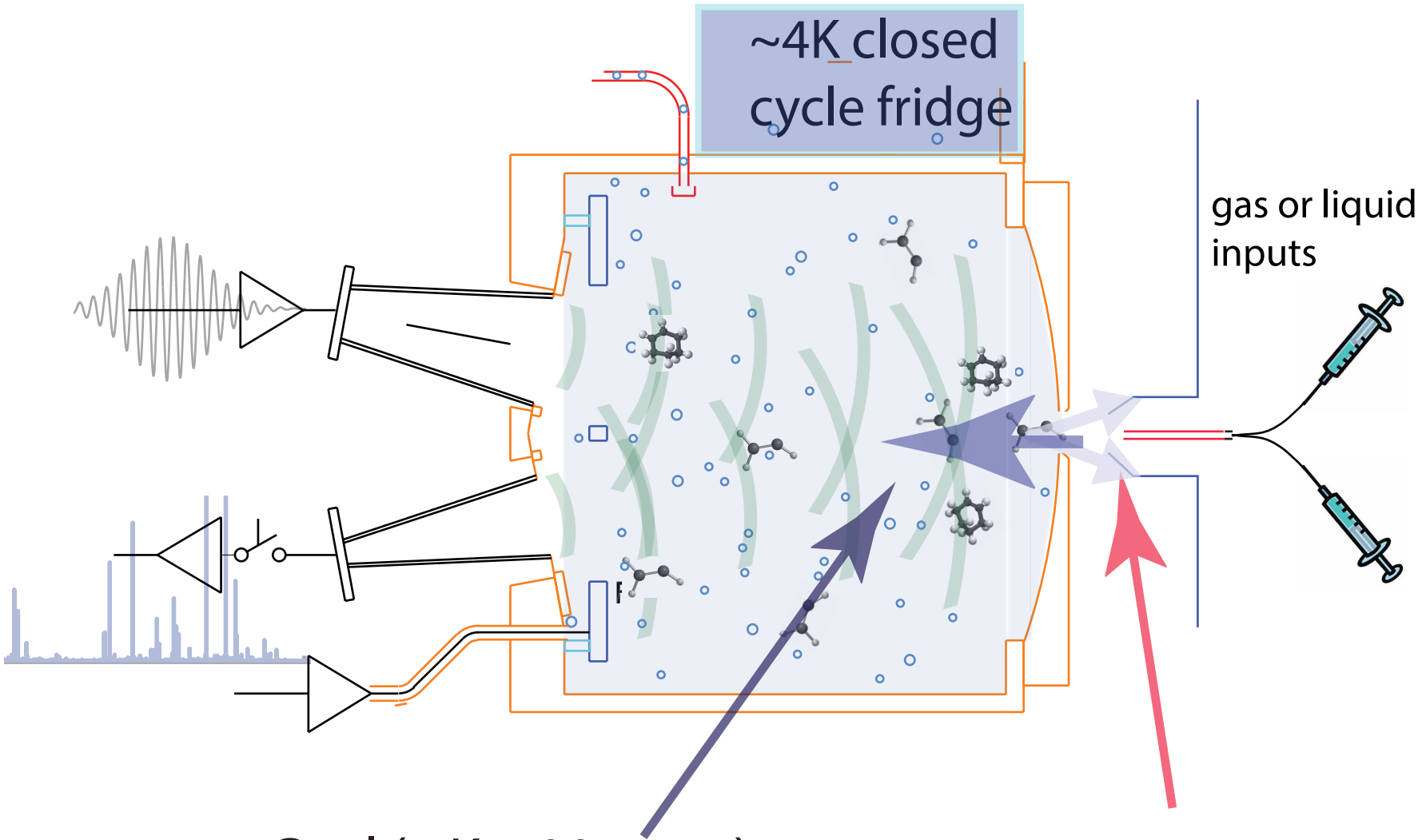
-Dark matter?



if cooling atoms is a good idea
..cooling molecules is a GREAT idea

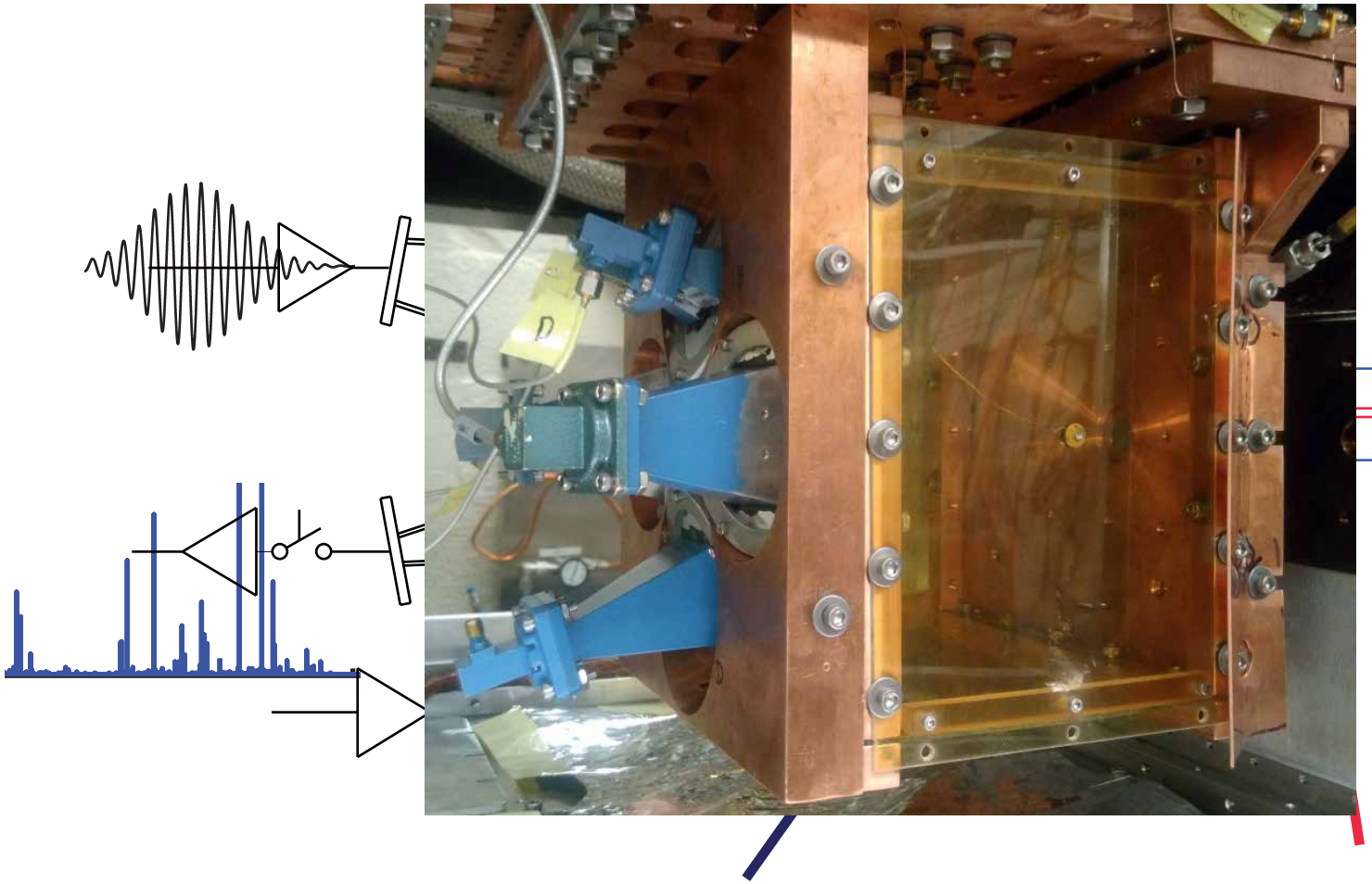


Our favorite (but unusual) source of cold molecules:



DeLucia, 1989
Doyle, 1995
Egerov, 2006
Campbell, 2008

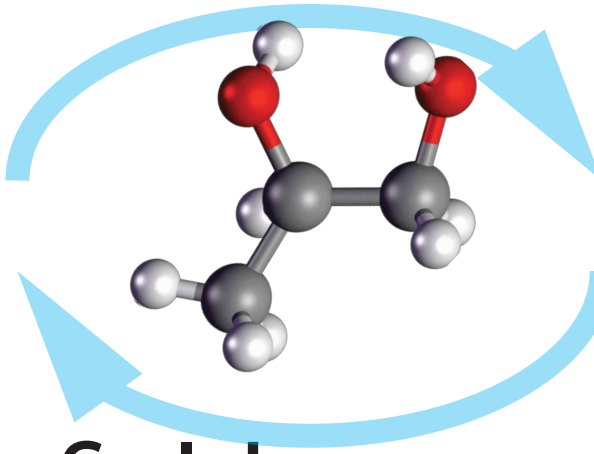
Our favorite (but unusual) source of cold molecules:



gas or liquid inputs

How to identify a polar molecule

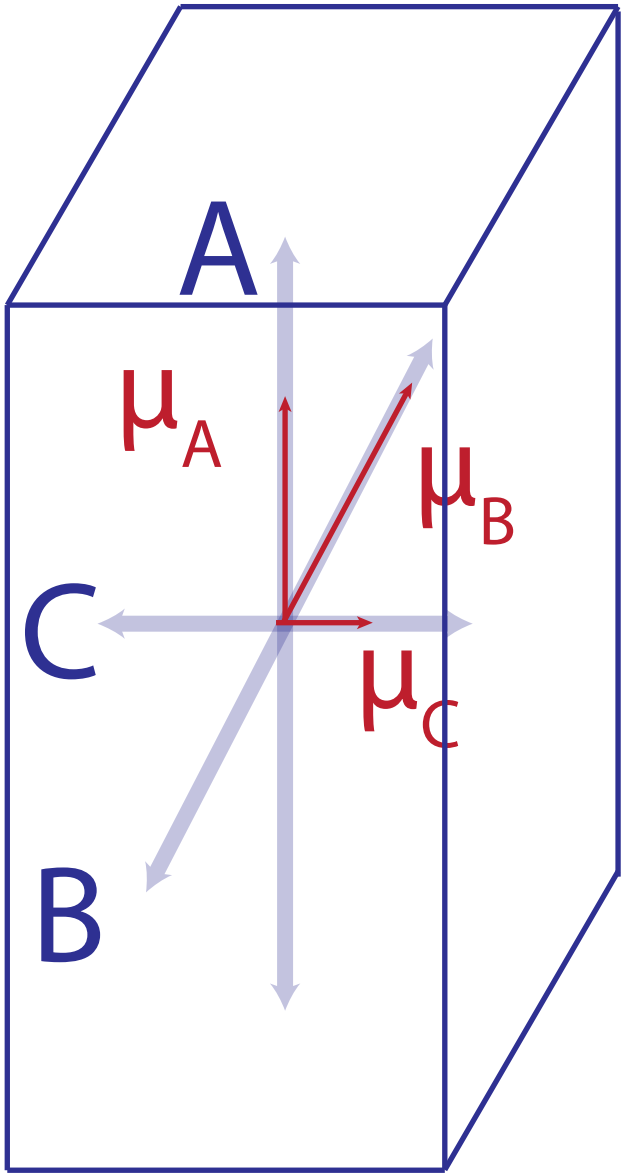
1: Stop its thermal rotation [cool it down]

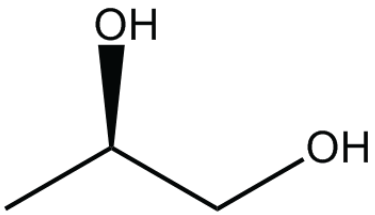


2: Kick it so it rotates

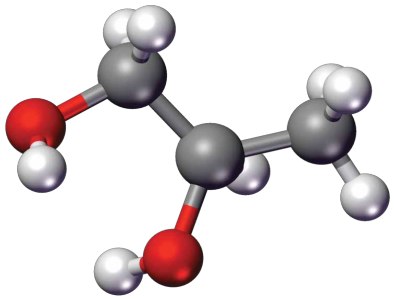
3: Record the resulting electric field

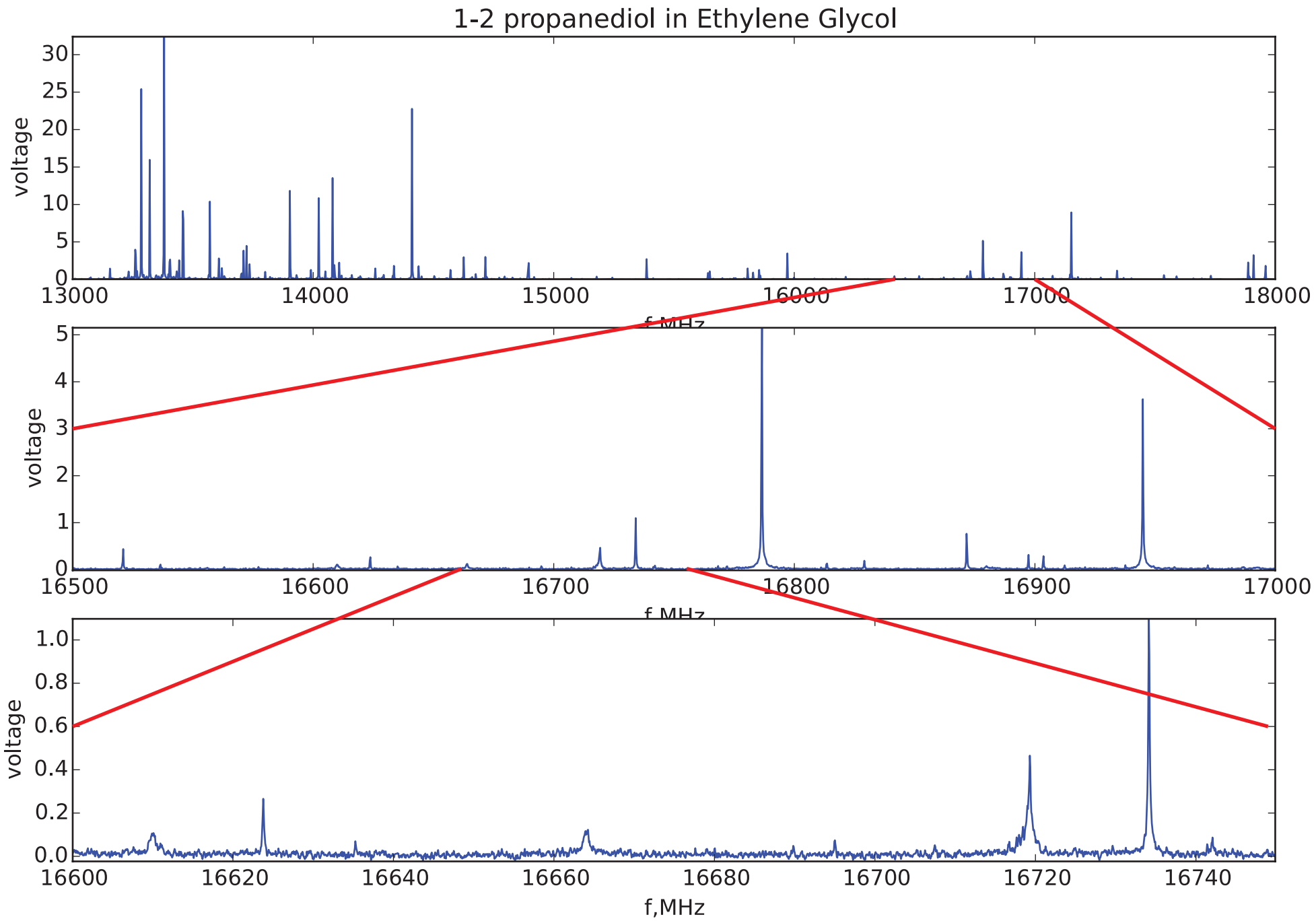
A microwave's view of a polar molecule



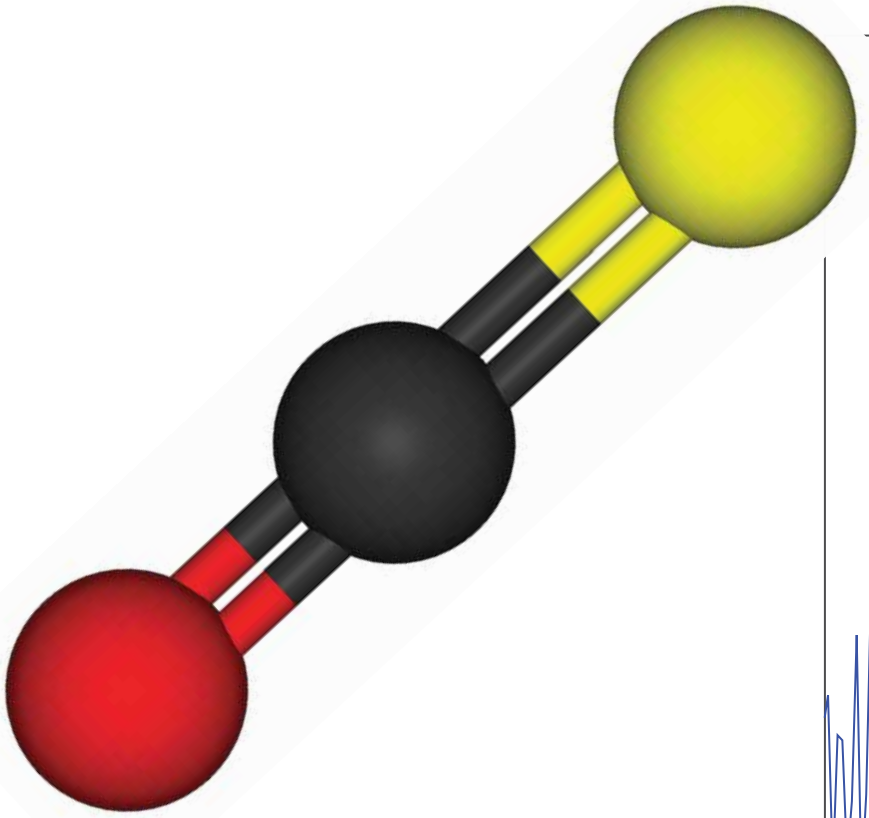


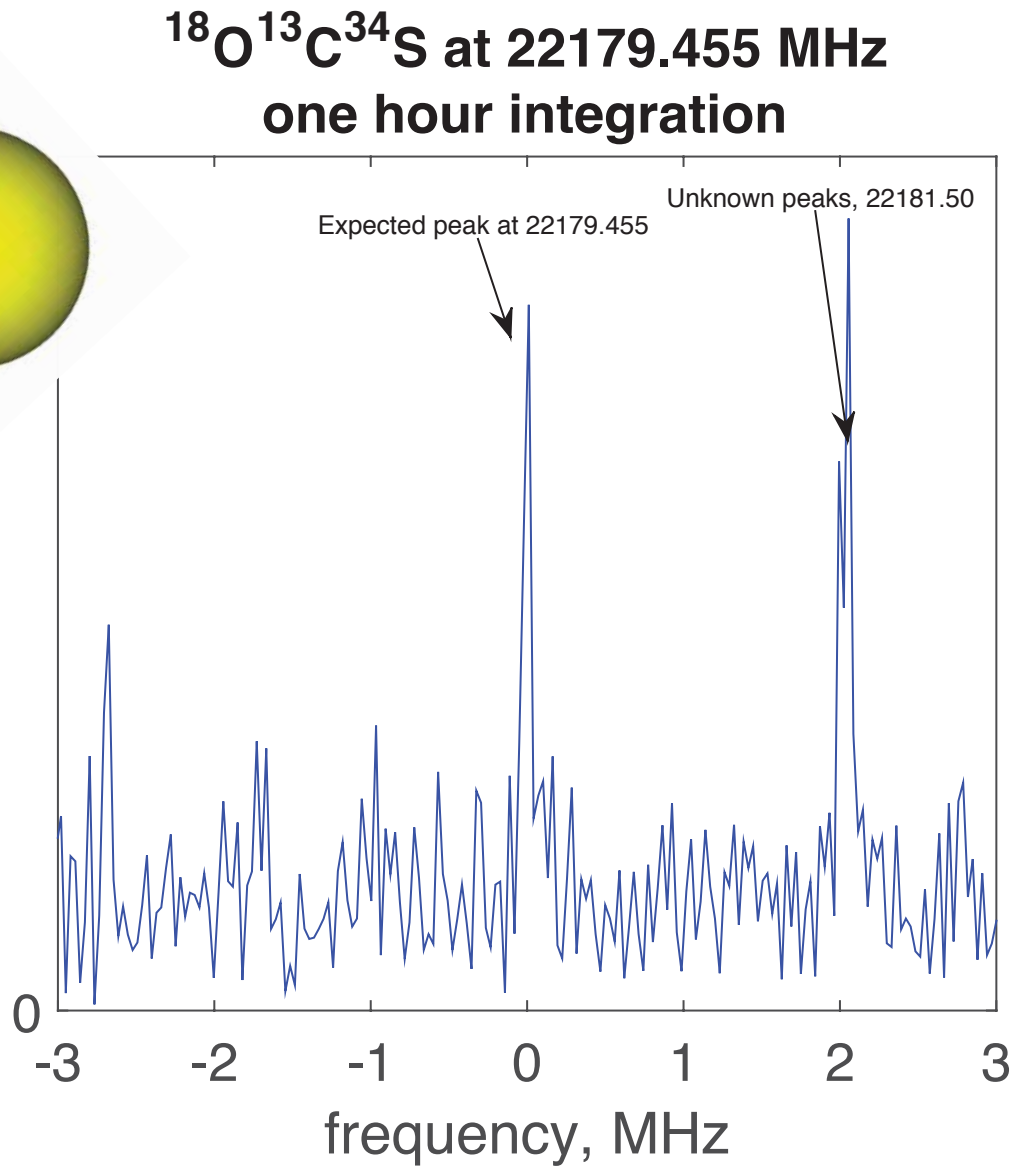
R 1,2-propanediol

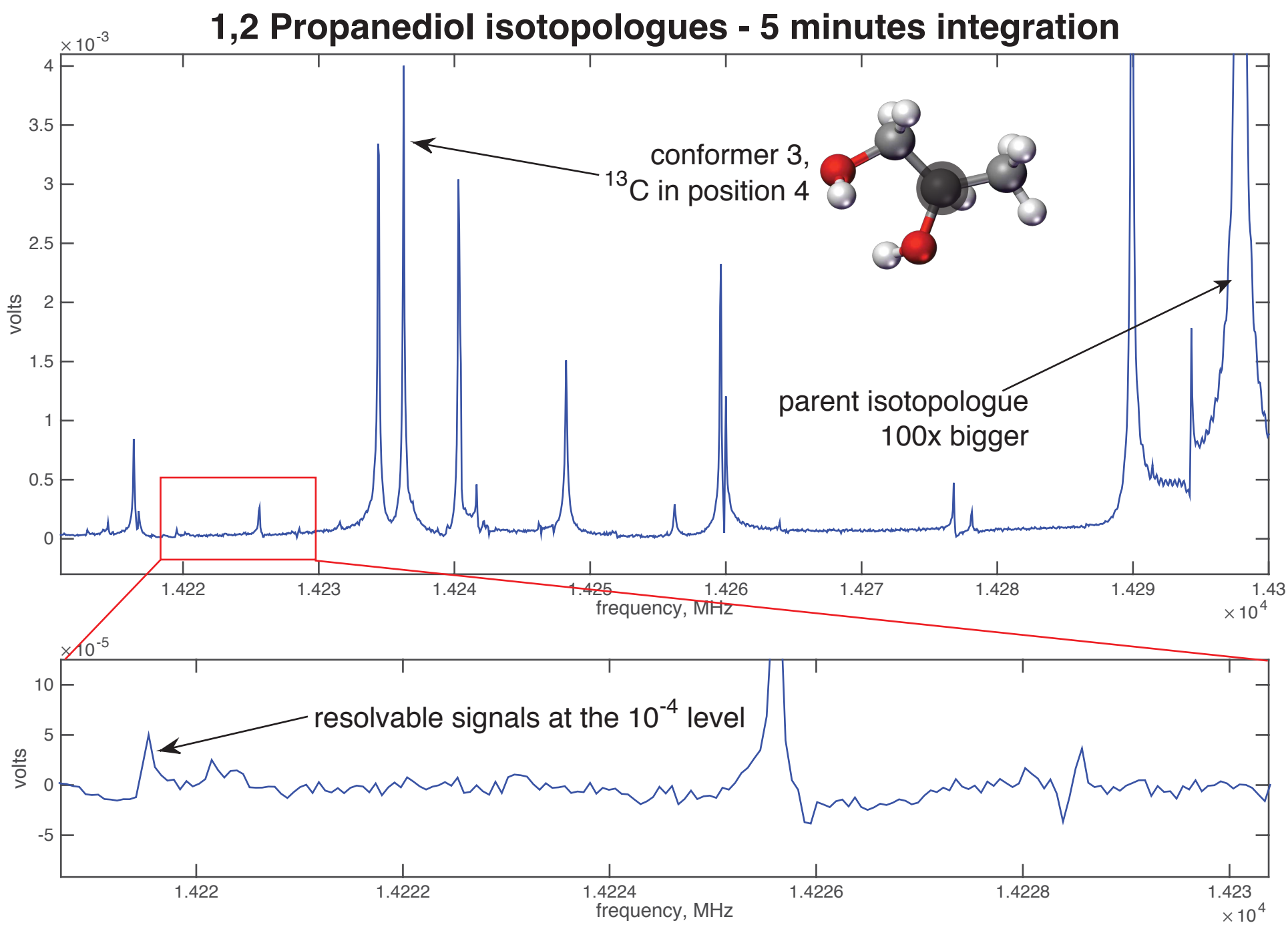



1-2 propanediol in Ethylene Glycol
voltage
30
25
20
15
10
5
0
13000
14000
15000
16000
17000
18000
f,MHz
voltage
5
4
3
2
1
0
16500
16600
16700
16800
16900
17000
f,MHz
voltage
1.0
0.8
0.6
0.4
0.2
0.0
16600
16620
16640
16660
16680
16700
16720
16740
f,MHz

Our high repetition rate (~50 kHz) and cryogenic noise temperature give us un-precedented sensitivity

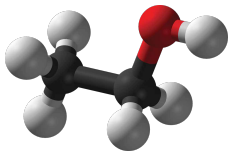




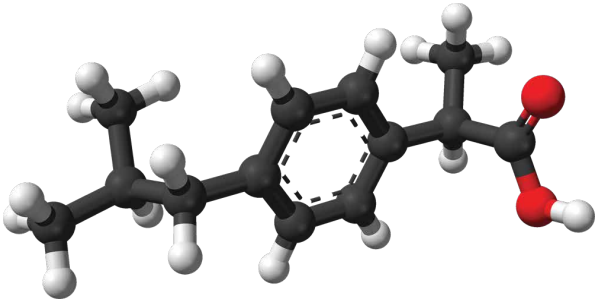

1,2 Propanediol isotopologues - 5 minutes integration
× 10^-3
4
3.5
3
2.5
2
1.5
1
0.5
0
volts
conformer 3,
13C in position 4
parent isotopologue
100x bigger
1.422
1.423
1.424
1.425
1.426
1.427
1.428
1.429
1.43
frequency, MHz
× 10^4
× 10^-5
10
5
0
-5
volts
resolvable signals at the 10^-4 level
1.422
1.4222
1.4224
1.4226
1.4228
1.423
frequency, MHz
× 10^4

The goal: determine the chemical structures in an unlabeled mixture

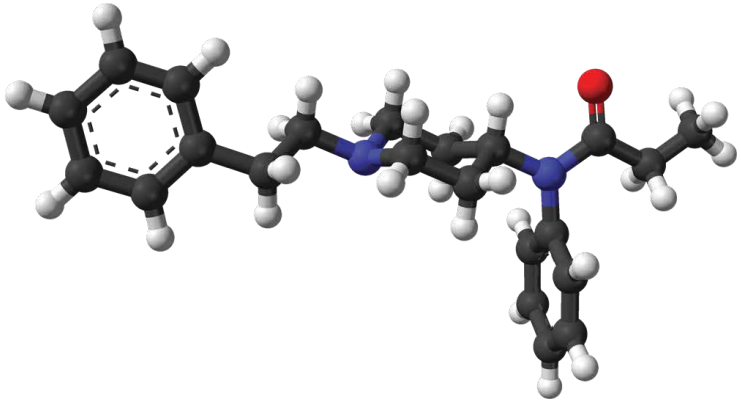
80%



15%

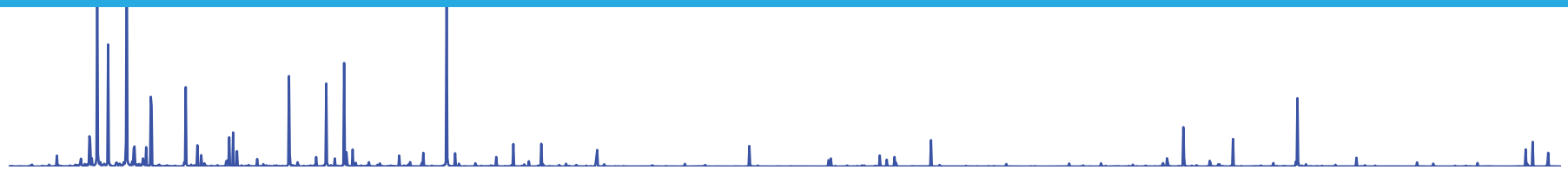


5%



We want to do this by measuring the x,y, and z position of each atom* in each molecule

What does a spectrum actually tell us?



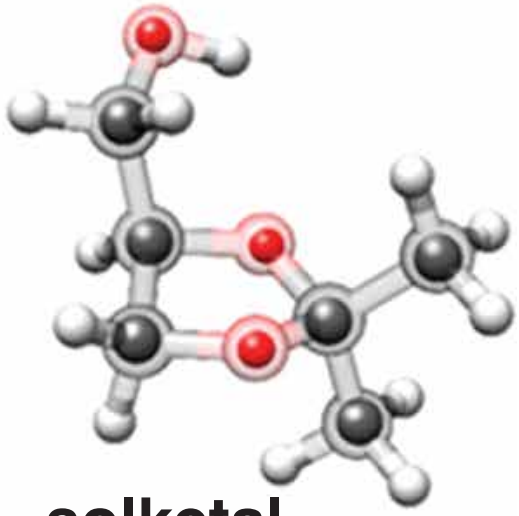
One isotopologue:

An unmistakable fingerprint, and internal motions

Each additional isotopologue:

the x,y,z location of that ^{13}C, ^{18}O, ^{15}N etc

This information is closer to x-ray diffraction than NMR:
If the ^{13}C spectrum can be seen, the position of every carbon in the molecule can be calculated

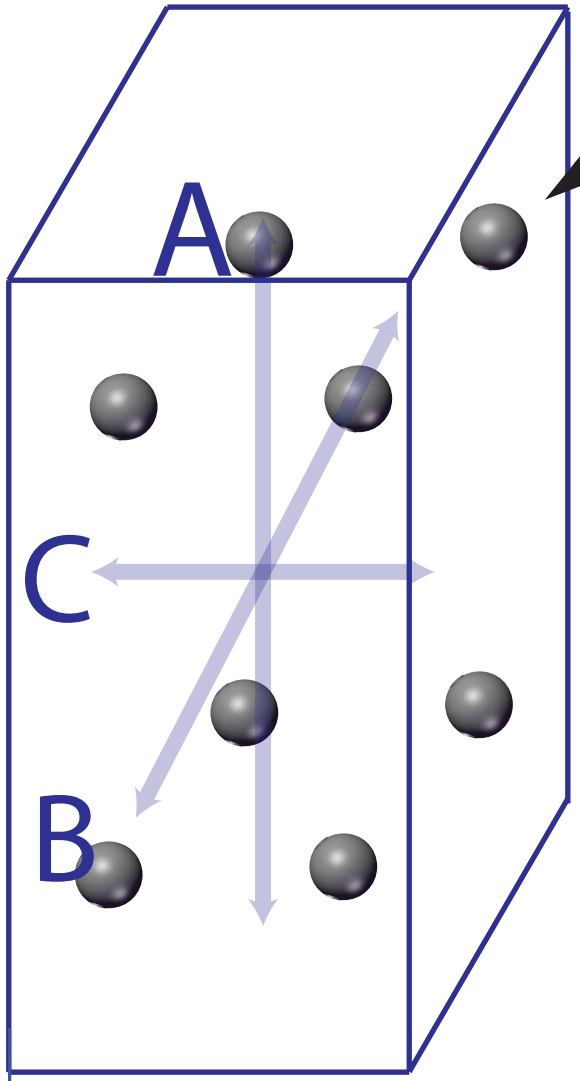


solketal

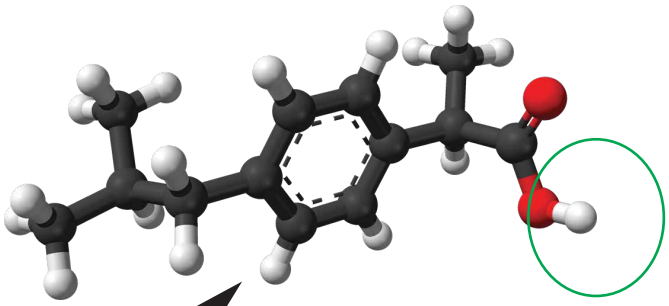
(2,2-dimethyl-1,3-dioxolan-4-yl-methanol)

From *Molecular Structure and Chirality Detection by Fourier Transform Microwave Spectroscopy*
S. Lobsiger, C. Perez, L. Evangelisti, K. Lehmann, Brooks H. Pate Physical Chemistry 2014

The natural abundance ^{13}C spectrum actually gives us |x|,|y|,|z| .. which is a good start but not enought go from a spectrum to a structure

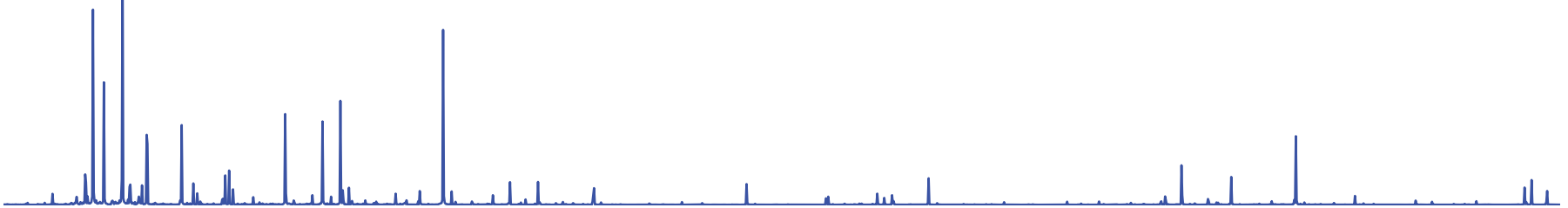


8 possible positions for each carbon

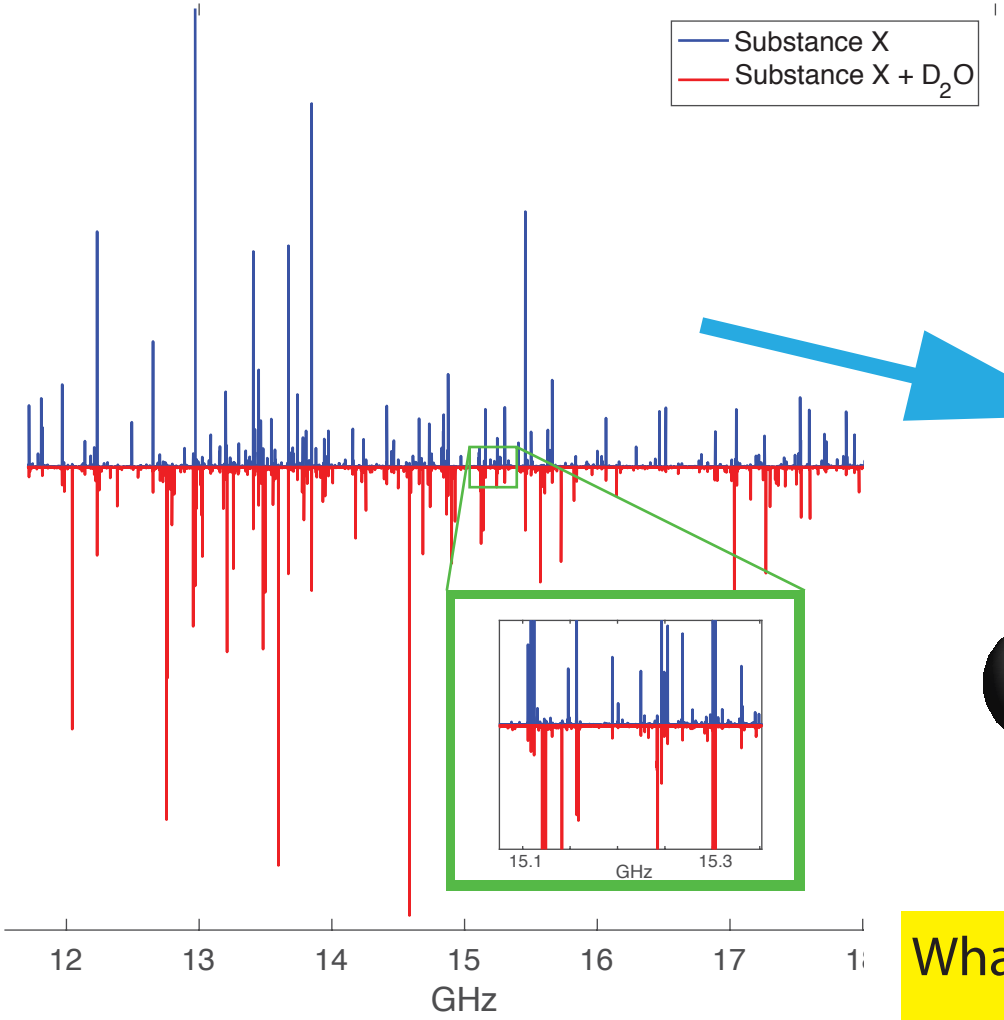


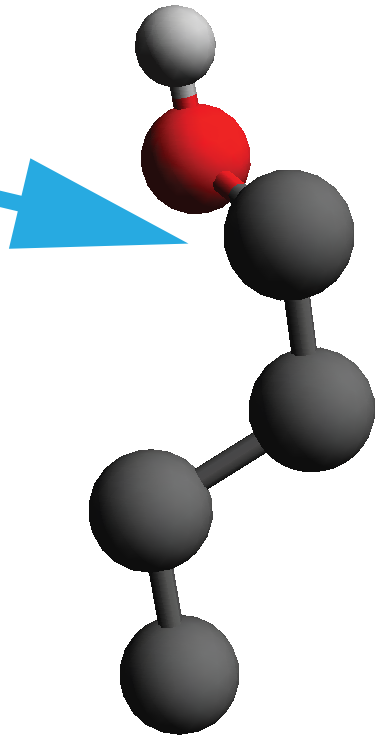
8^{12} "possible" structures

-but double substitutions would resolve them

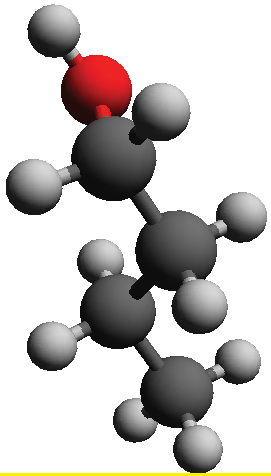


By looking at correlations in conformers and double substitutions, we have resolved our first structures with no prior knowledge





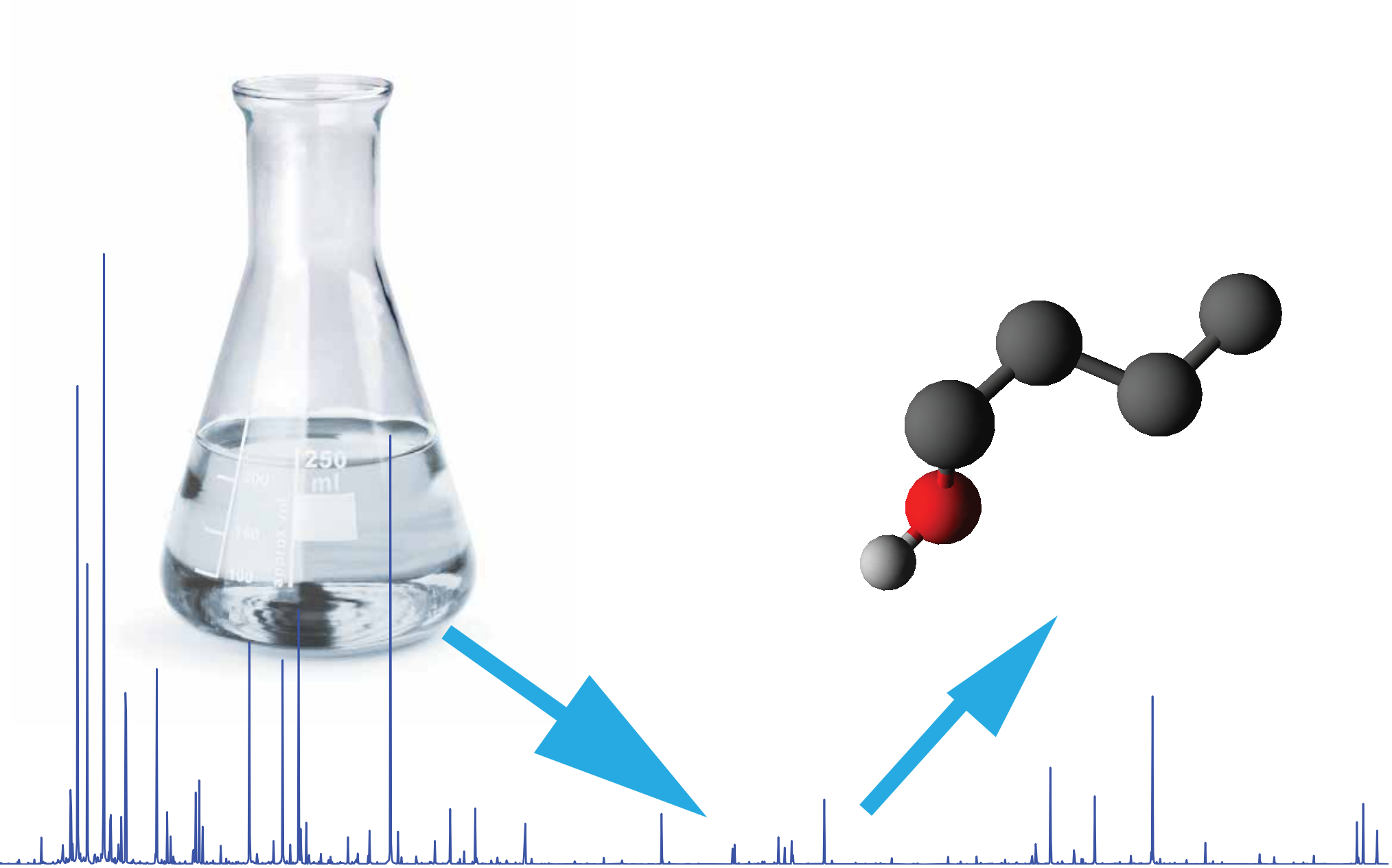
What we calculated



Actual structure

-Didn't tell it chemical composition
-No knowledge of physical chemistry (length of a C-C bond, etc)
-Haven't yet done a true 'blind' test - we knew what was in the bottle, even if the computer didn't

We’re getting there!

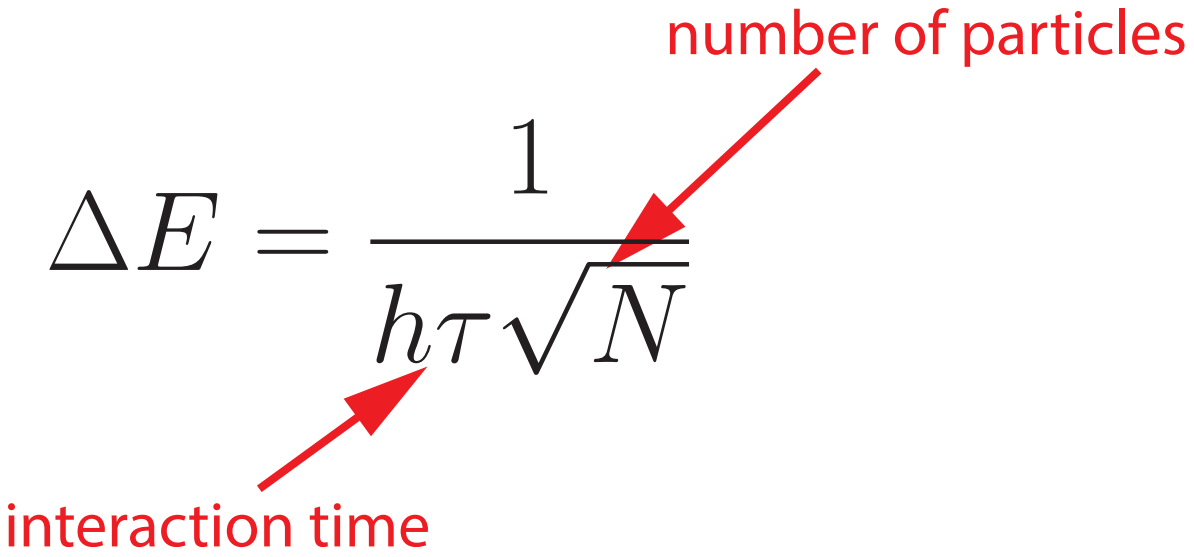


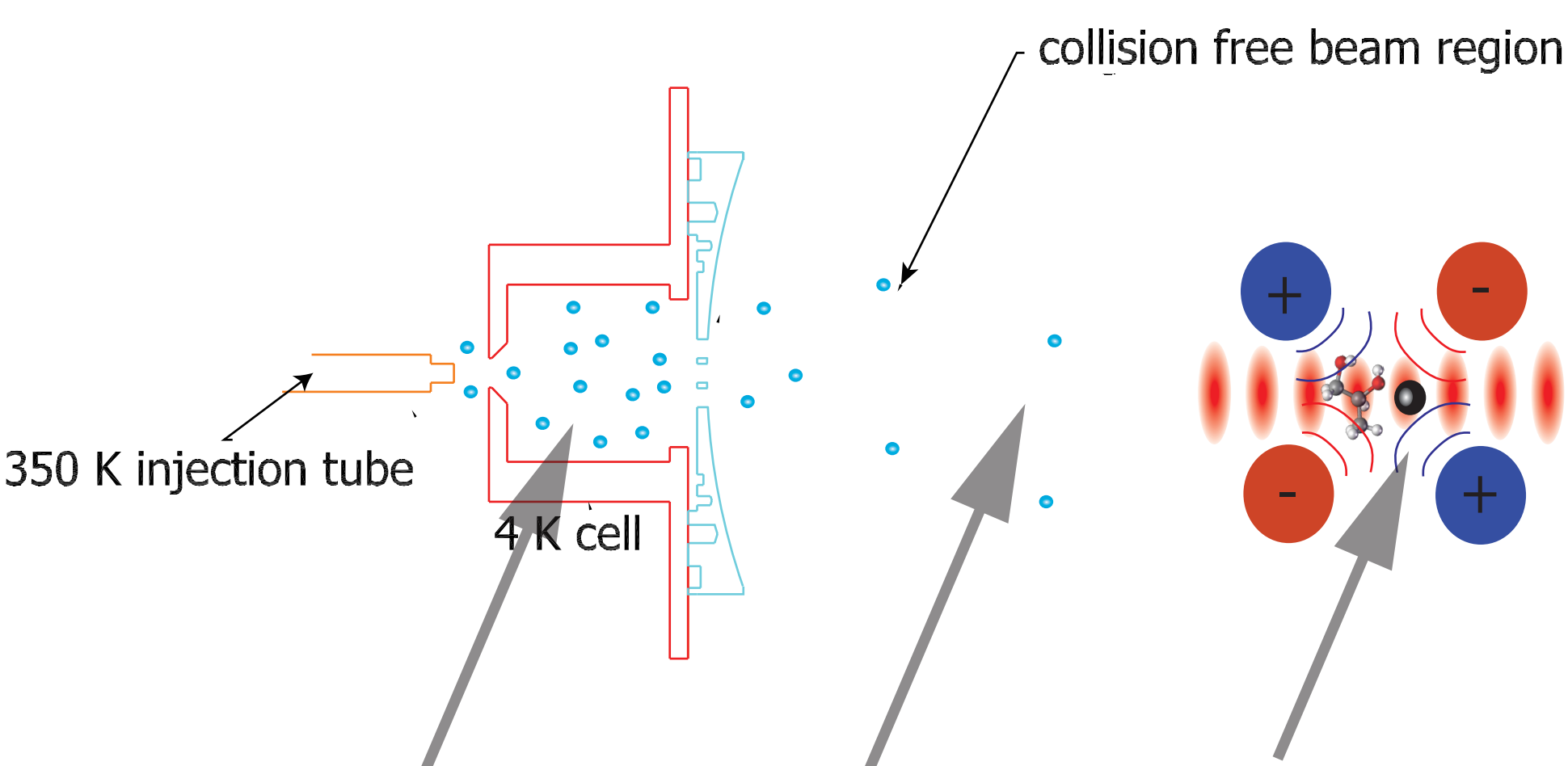
Can we use *spectroscopy* to search for BSM physics?

The basic idea:

Find two spectral lines which the standard model says are equal

Compare them with phenomenal accuracy





In cell:
$N = 10^{14}$
$T = 10^{-5}$ s

In beam:
$N = 10^{8}$
$T = 10^{-2}$ s

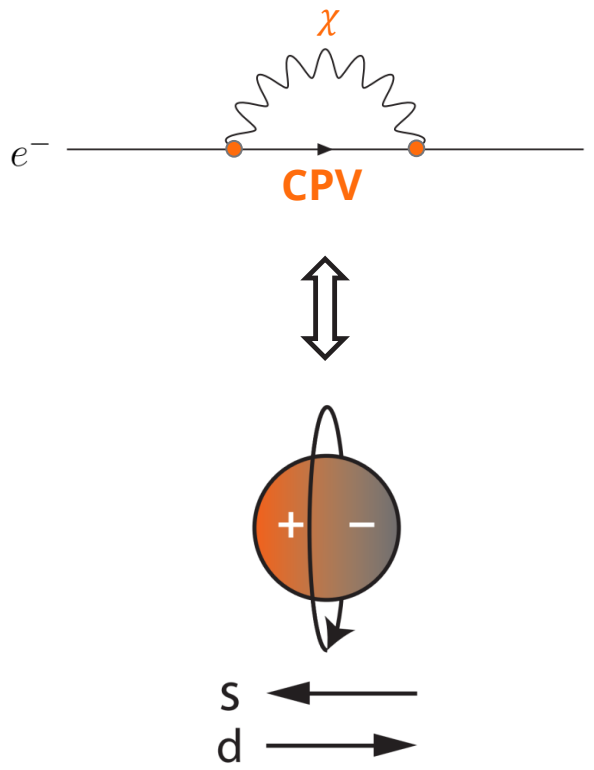
In trap:
$N = 10^{3}$
$T = 1$ s

$$\Delta E = \frac{1}{h\tau\sqrt{N}}$$

Nick Hutzler (Caltech) is driving this field in the "new molecule" direction

CP Violating Observables

- New CPV physics creates CPV observables at **low energies**
  - (Also high energies)
- Classic example: permanent electric dipole moments (EDMs)
  - **The existence of EDMs requires CPV**



Pathway to PeV Physics

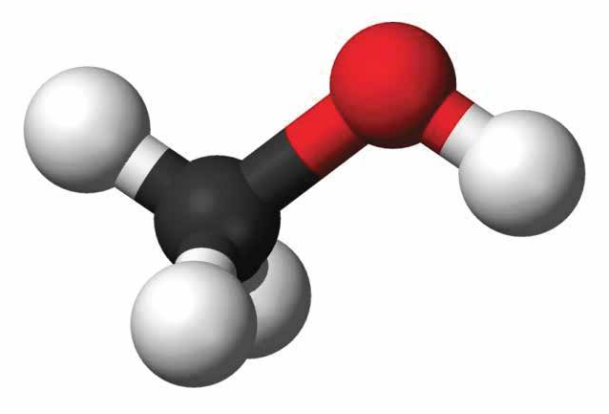
Feature	ThO, TaN	(Yb,Ba, Ra,Tl)F	WC	$(Hf,Th)F^+$	Hg,Ra, Cs,Rb	**Polyatomics**
Laser cooling	✗	✓	✗	✗	✓	✓
Full polarization	✓	✗	✓	✓	✗ ✗	✓
Internal co-mag.	✓	✗	✓	✓	✗	✓
>1 s lifetime	✗	✓	✓	✓	✓	✓
Scalable (Large #)	✓	✓	✓	✗	✓	✓

I. Kozyryev and NRH, Phys. Rev. Lett. 119, 133002 (2017)

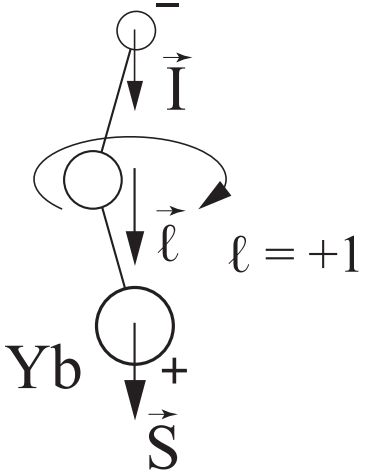
- Realistic pathway to PeV-scale physics
- General approach, applicable for many measurements
  - Electron EDM: YbF → YbOH, BaF → BaOH, …
  - Nuclear Schiff: TlF → TlOH, RaF → RaOH, …
  - Nuclear Anapole: BaF → BaOH, …

Molecules have lots of sleeves..

..and lots of tricks up their sleeves



Methanol - m_p/m_e



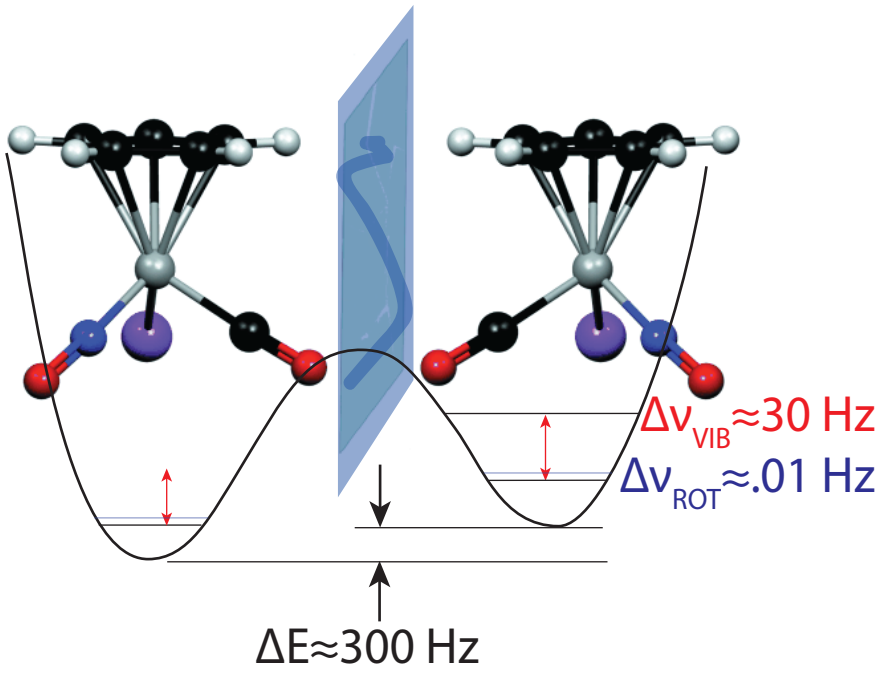
v = 1 YbOH - eEDM

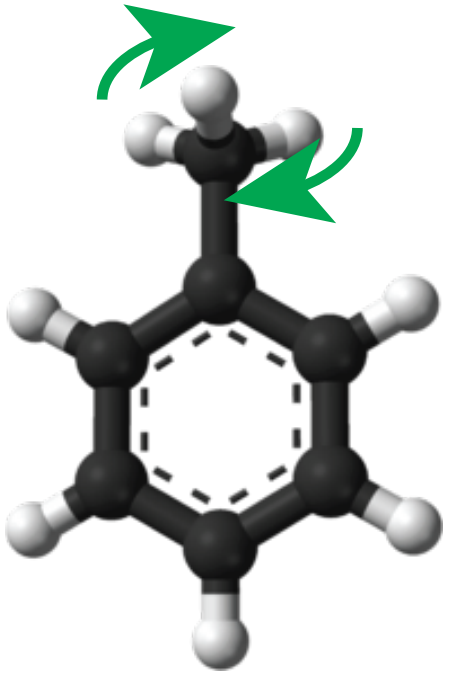
Anticipated resolution (rotational or vibrational transitions

~100 Hz for polar ions

~< 1 Hz for non-polar ions

Chirality gives us other 'nearly symmetric' states - are there remotely plausible BSM models that predict shifts?

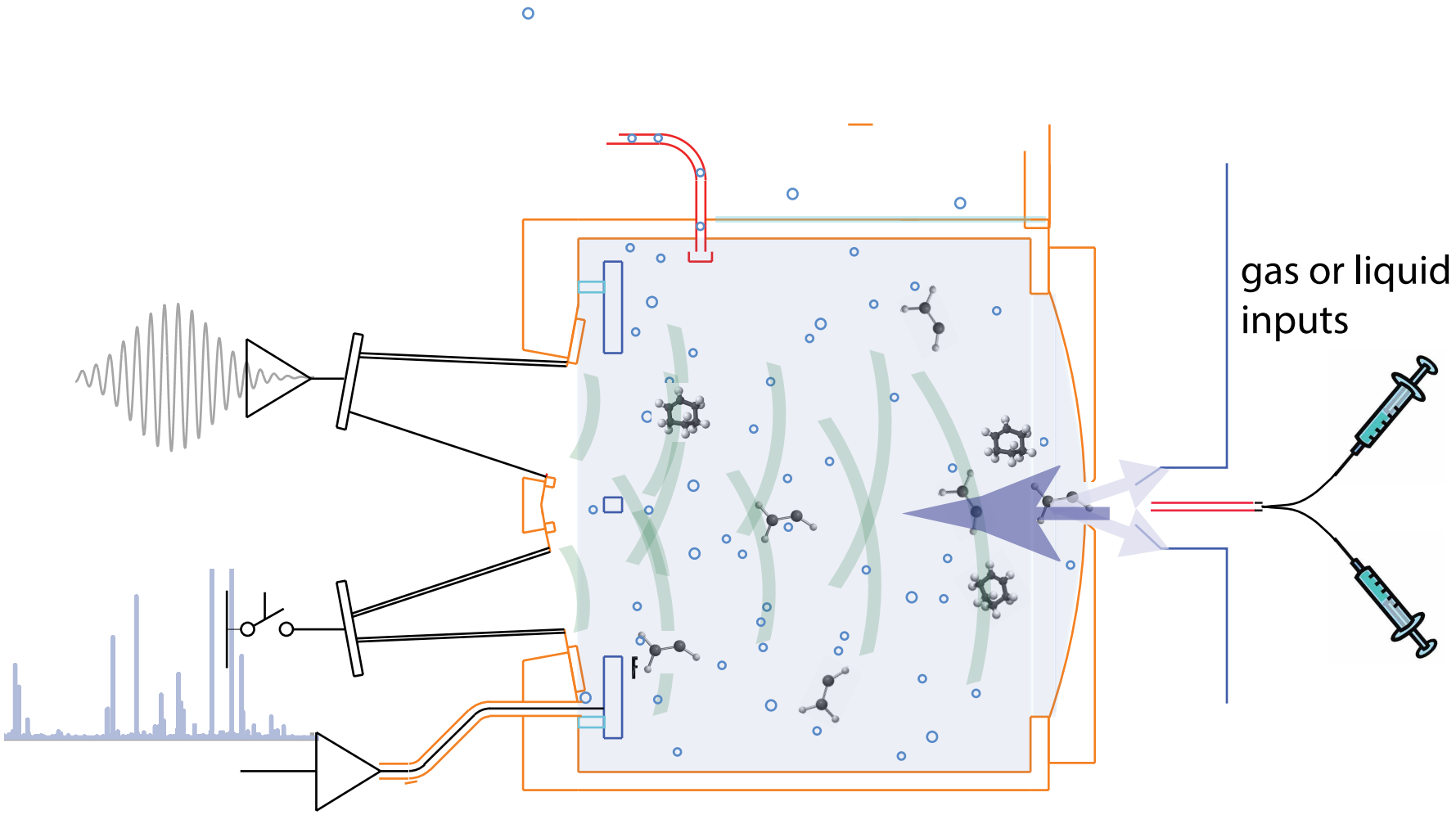




"kinetically" chiral molecules?

(please somebody give me a reason to purify this!)

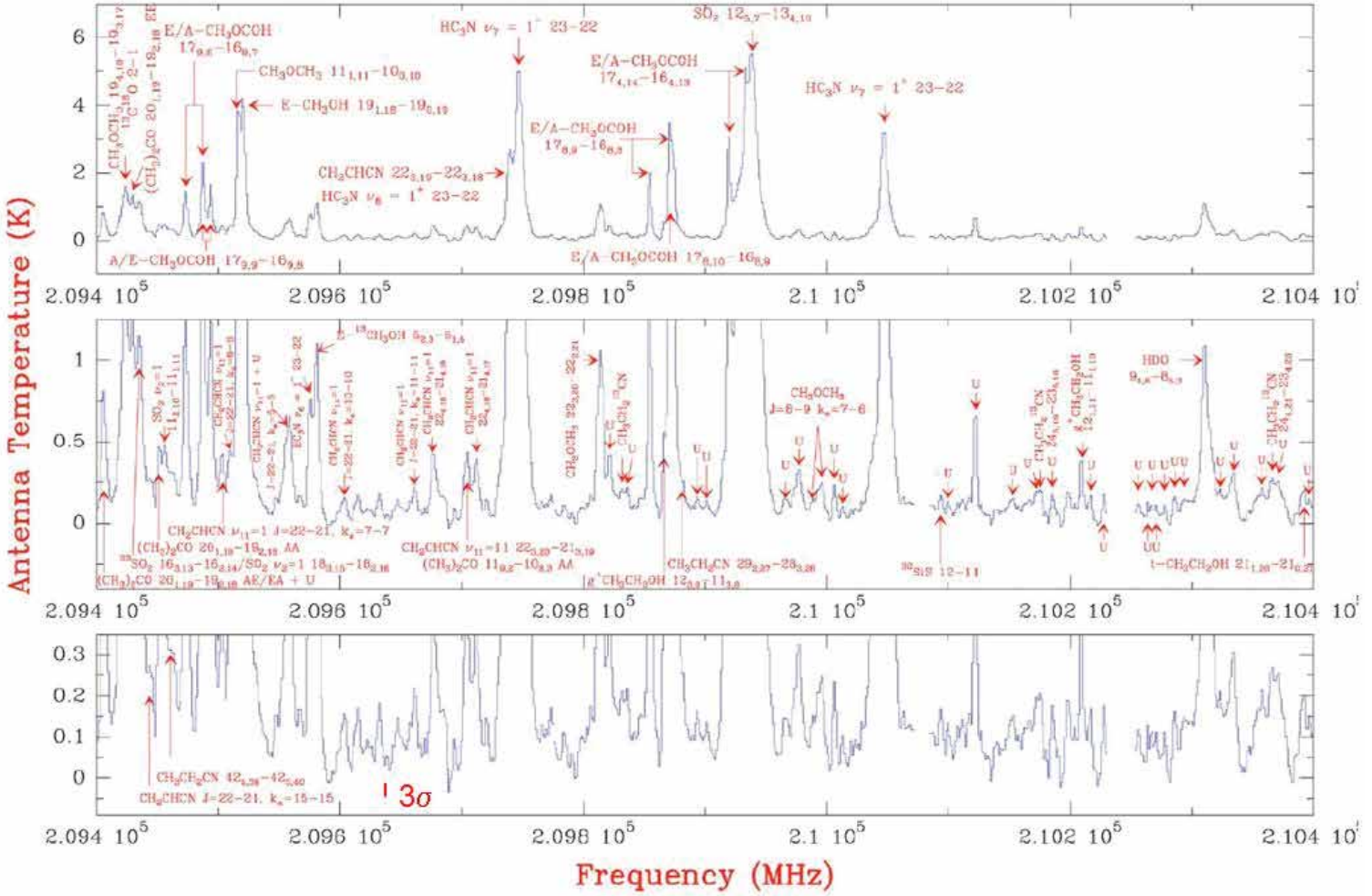
Can we use cold molecules for direct detection dark matter searches?



And now for some wild speculation..

I googled "what would happen if.." and got an amazing number of apocalyptic astronomical responses. This image came from "Business Insider" magazine, in an article exploring "what would happen if Earth stopped rotating?"

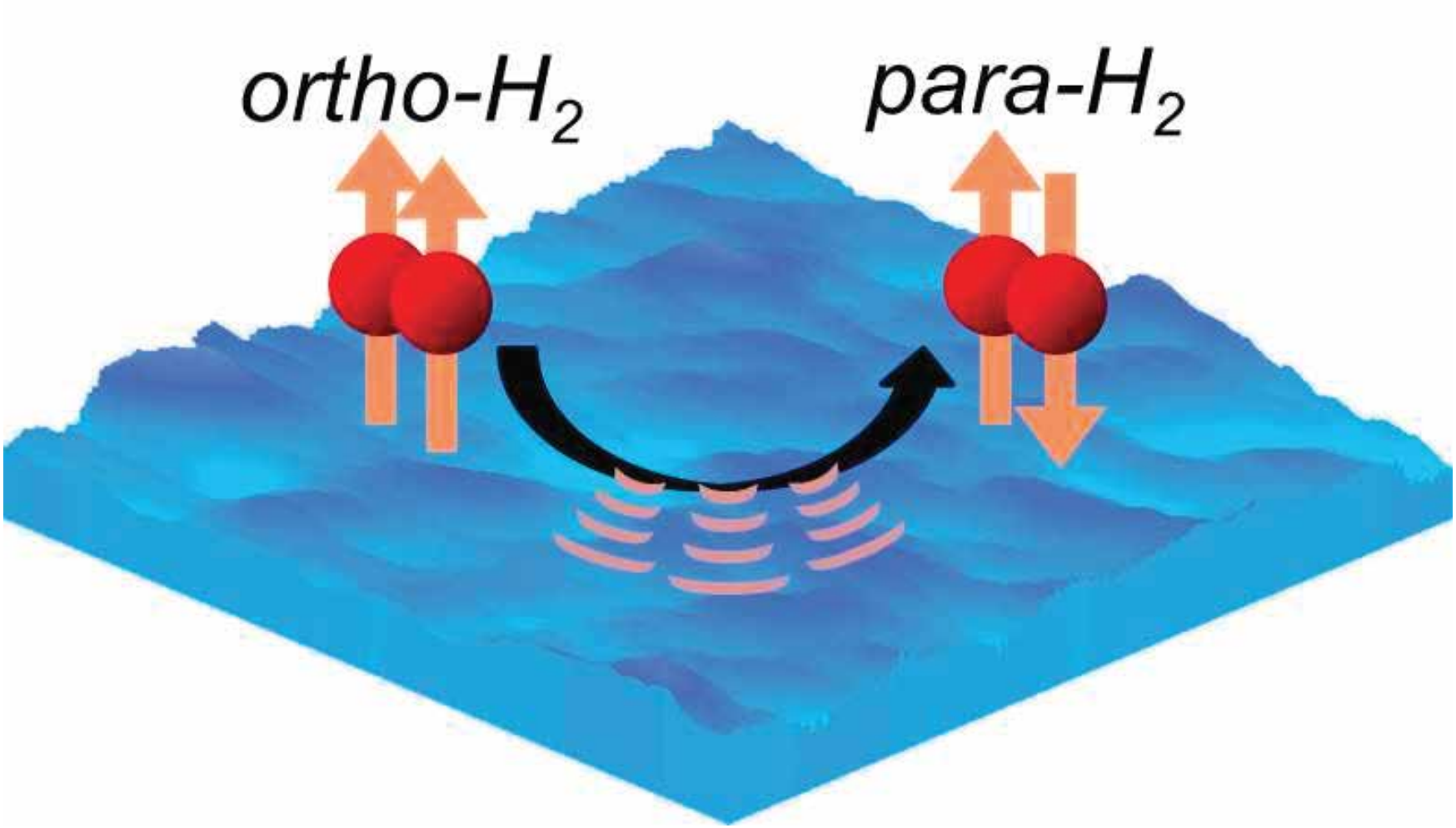
Can we use astrochemical molecules for direct detection dark matter searches?



LINE CONFUSION LIMIT REACHED. WHAT TO DO ?
ALMA WILL BE 8 times more sensitive than the 30-m radio tele

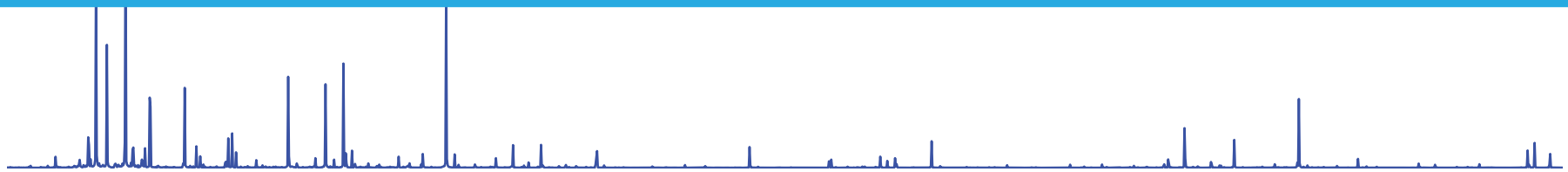
A coherent DM “wind” looks a lot like Lorentz variance - can we see a spectral “preferred” velocity?

What are the selection rules for DM+molecule collisions?



Natural (radiative) lifetime is “Aeons” - at least 160,000 years

What does a spectrum actually tell us?



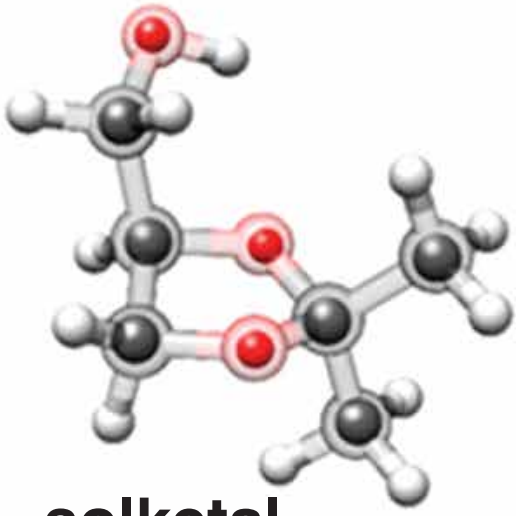
One isotopologue:

An unmistakable fingerprint, and internal motions

Each additional isotopologue:

the x,y,z location of that ^{13}C, ^{18}O, ^{15}N etc

This information is closer to x-ray diffraction than NMR:
If the ^{13}C spectrum can be seen, the position of every carbon in the molecule can be calculated



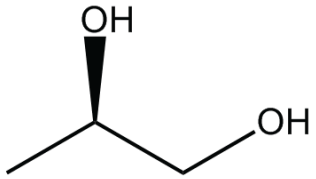
solketal

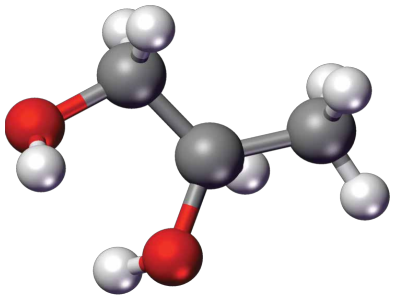
(2,2-dimethyl-1,3-dioxolan-4-yl-methanc

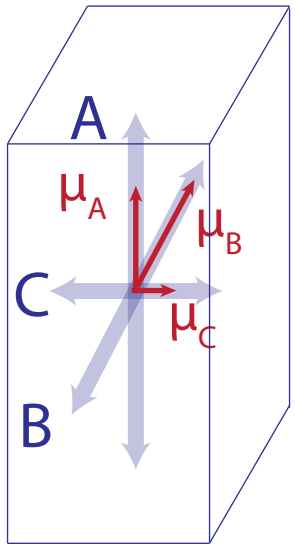
From *Molecular Structure and Chirality Detection by Fourier Transform Microwave Spectroscopy*
S. Lobsiger, C. Perez, L. Evangelisti, K. Lehmann, Brooks H. Pate Physical Chemistry 2014

The Hamiltonian of a chiral asymmetric top is enantiomer dependent

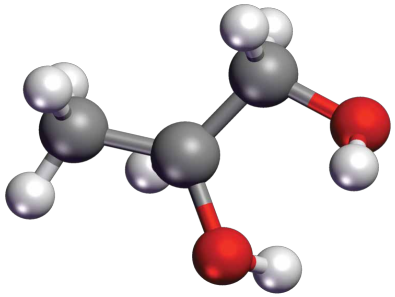
R 1,2-propanediol

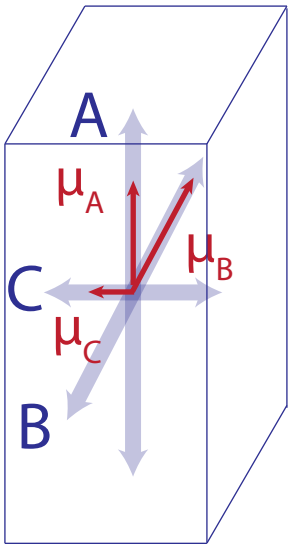


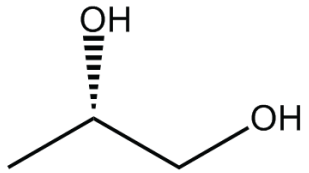




S 1,2-propanediol

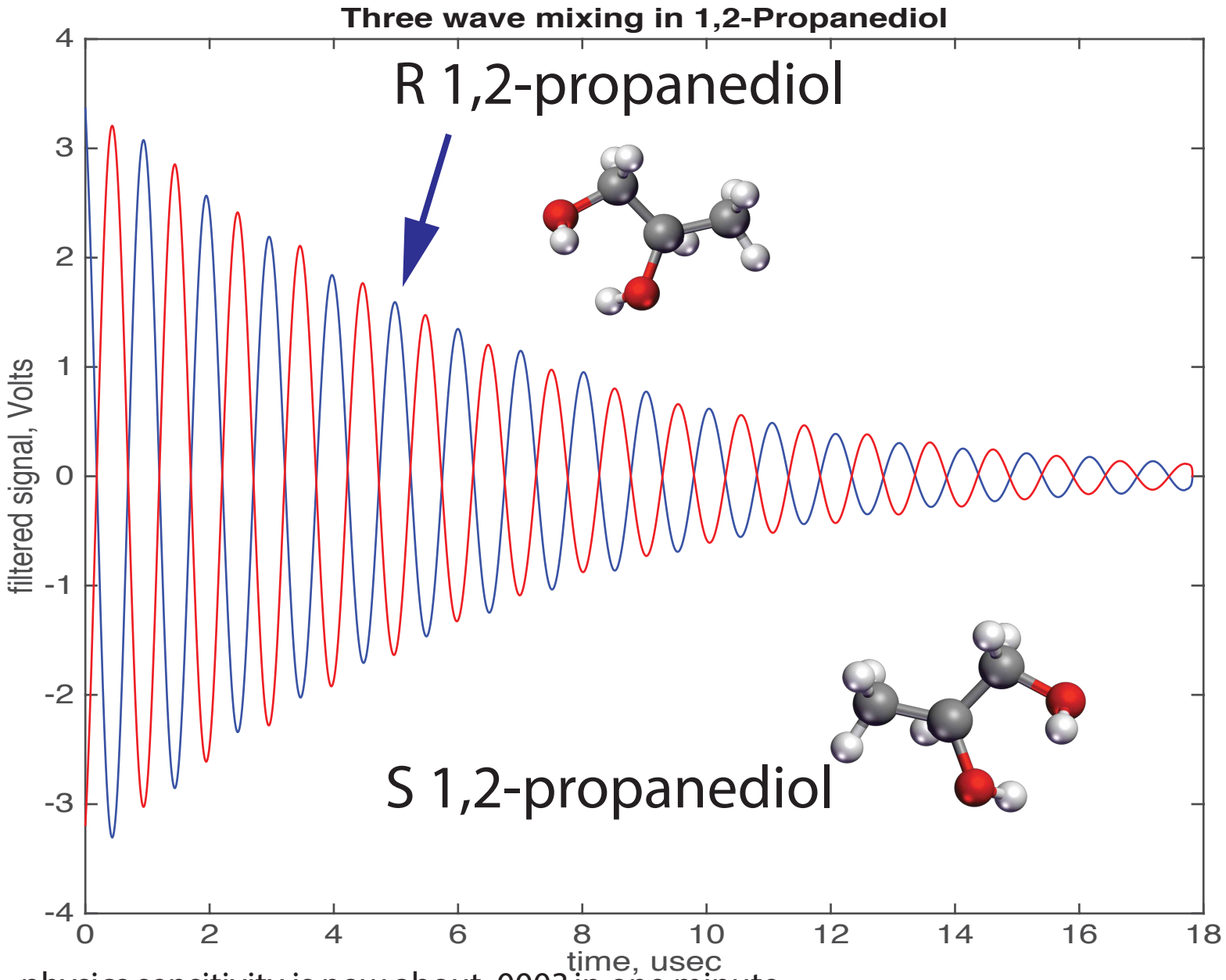






Opposite enantiomers have:
The same rotational constants A, B, and C,
The same magnitude of dipole moment components $|\mu_a|$, $|\mu_b|$, and $|\mu_c|$,
Opposite sign of the combined quantity $\mu_a\mu_b\mu_c$ (independent of choice of axes)

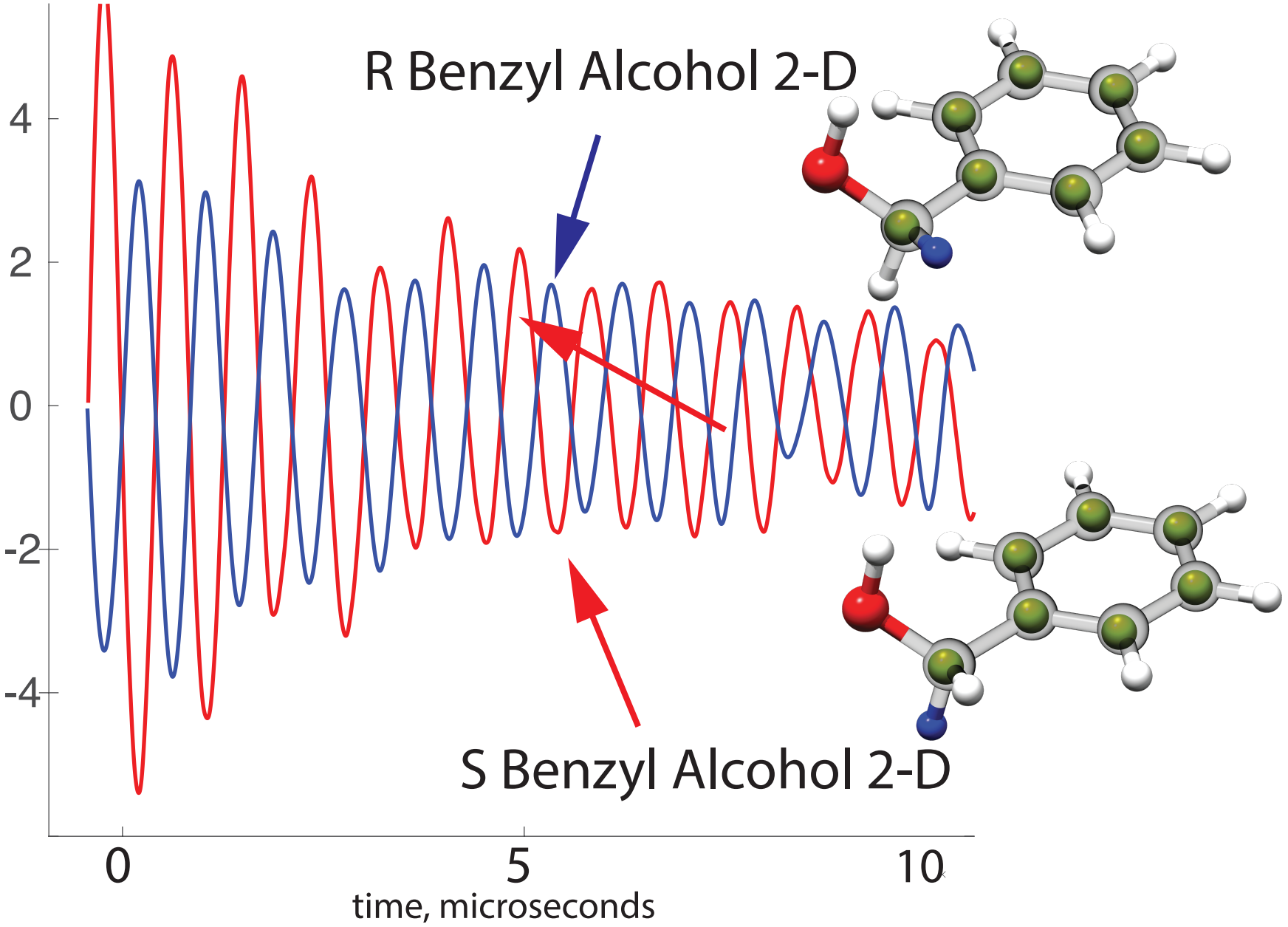
We can see chirality too:



physics sensitivity is now about .0003 in one minute

..cleanliness is an issue

This is a purely geometric - not electronic - effect;
we can see chirality in subtances that are just chiral by isotope



See talk by Lincoln Satterthwaite, 8 pm tonight!

Between 1-D microwave spectroscopy, NMR, and three wave mixing, we have a “zero entropy” picture of this molecule