High resolution rotational spectroscopy of HCSSH: a CS_2 proxy in the ISM

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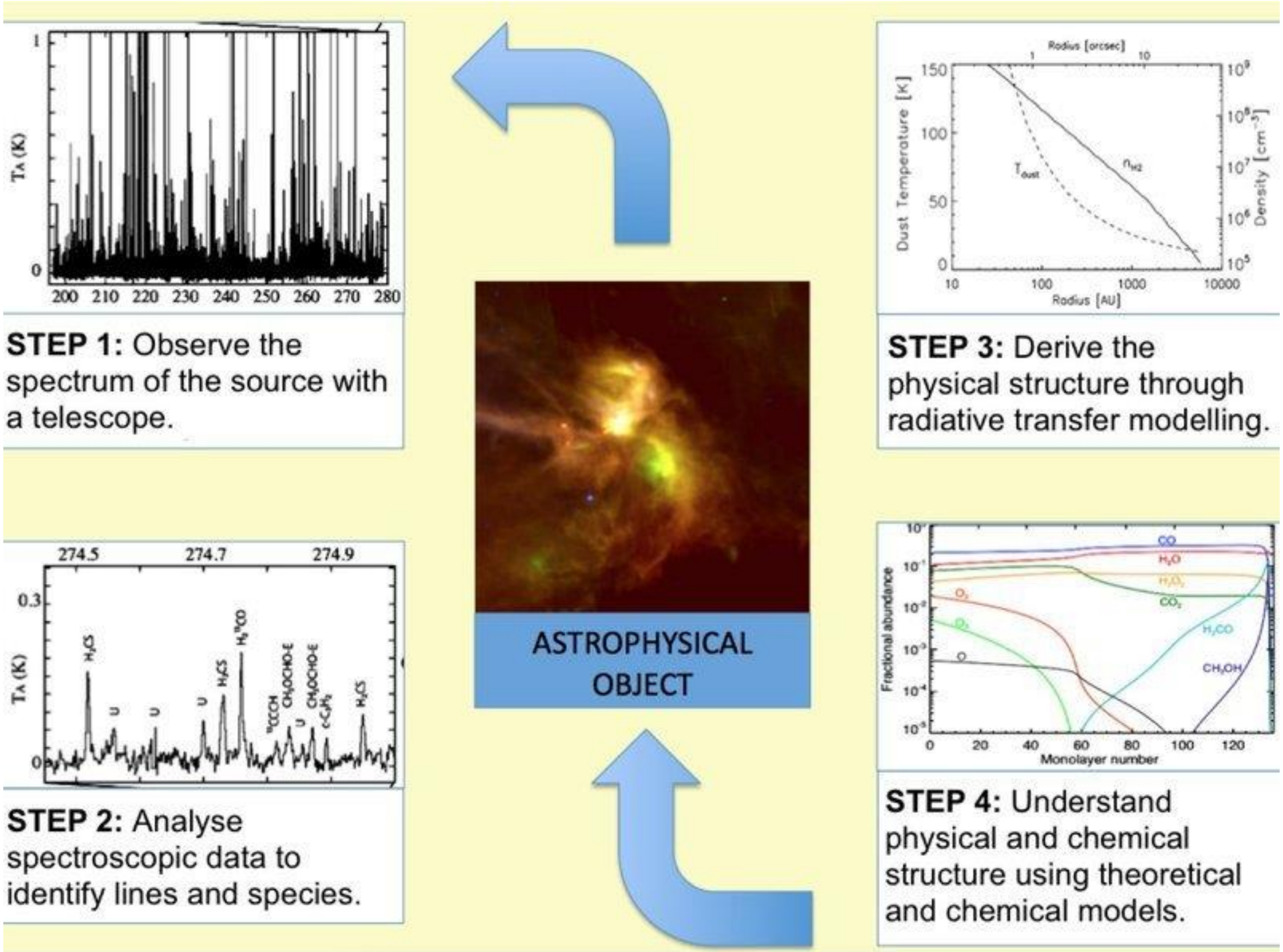


Laboratory studies give large pools of spectra

Important Tracers for Astrochemistry

- Abundant stable species
  e.g. CO, NH_3, etc.
- Unstable molecules (free radicals)
  e.g. $CN^{\cdot}$, $HCO^{\cdot}$, $CH_3O^{\cdot}$, etc.
- Protonated species and derivatives of non-polar molecules
  e.g. N_2H^+, $HOCO^+$, $HCOOH$ etc.

Sulphur bearing compounds

Sulphur Depletion Problem

S-bearing molecules detected in the 70s:

CS, OCS, H_2S, H_2CS, SO, SO_2, SiS,
NS, CH_3SH, HNCS

Observed abundances lower than
observed cosmic abundance
in molecular clouds

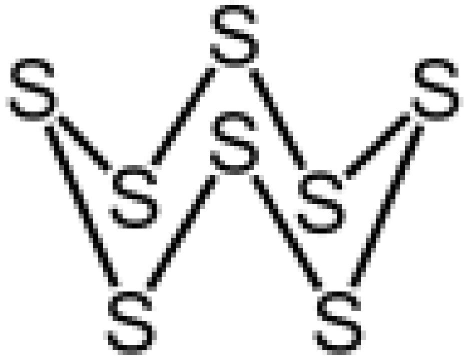
WHY?

Sulphur Depletion Problem

Sulphur depleted on grains as:

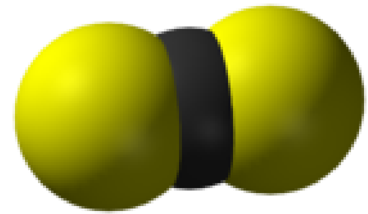
-Polysulphanes, H_2S_n (e.g. HSSSH)

-Sulphur polymers, S_n (e.g. S_8)



Wakelam et al. 2004

CS_2 – Gas-phase sink of sulphur

S=C=S 

Detected in comets’ comas,
but not in the ISM <u>because</u>:

-No permanent electric dipole moment

(Impossible Radio-telescopes detection)

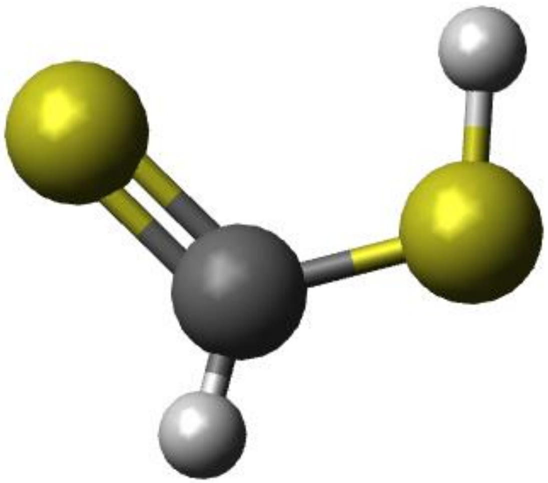
-Infrared features overlap with other signals

(Difficult Interstellar Ices detection)

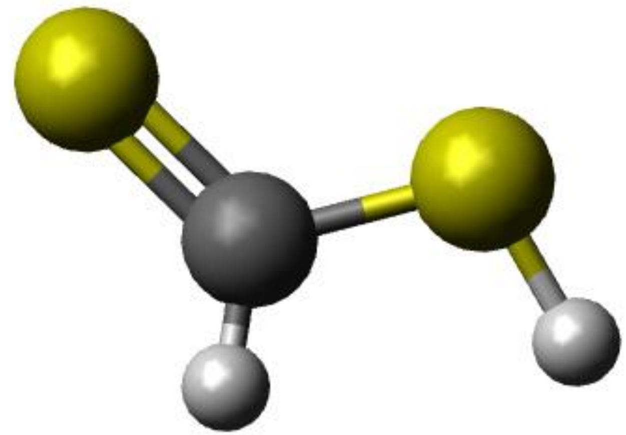
Garozzo et al. 2010

$HCSSH$ - Dithioformic acid

Chemically related to CS_2



trans



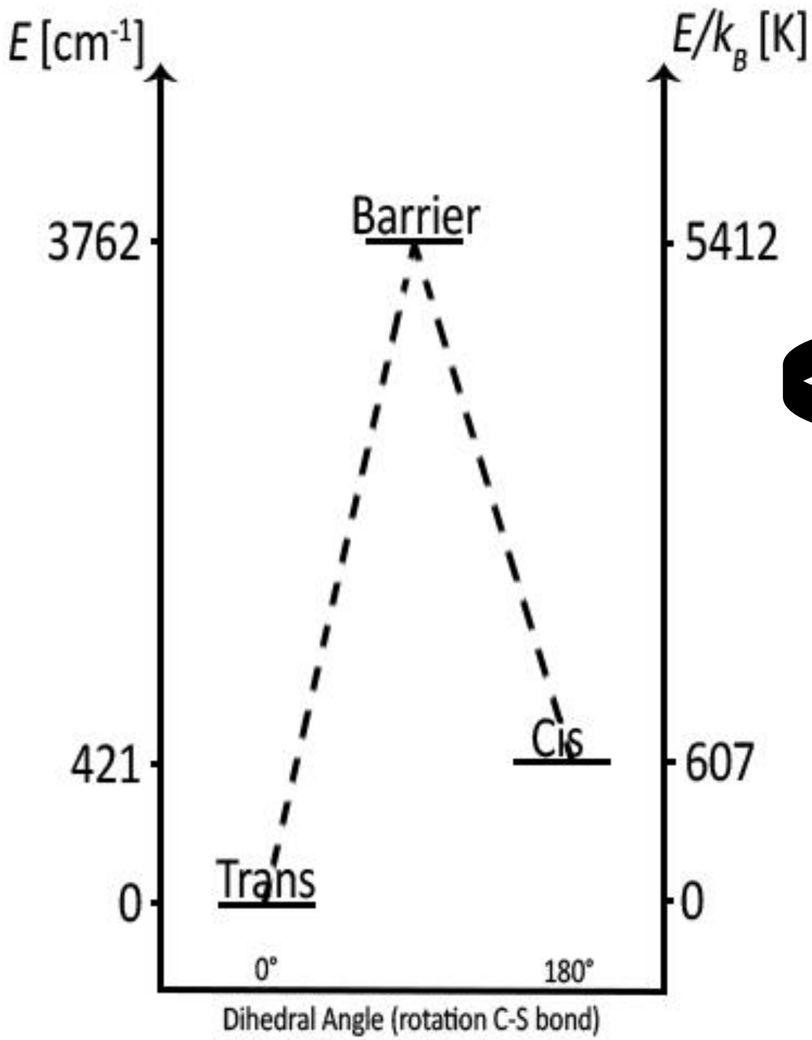
cis

2 conformers - near-prolate asymmetric rotors

μ_a = 1.53 D	**μ_a = 2.1 D**
μ_b = 0.19 D	μ_b = 1.67 D

Previous study by Bak et al. (1978) in the cm range (18 – 40 GHz)

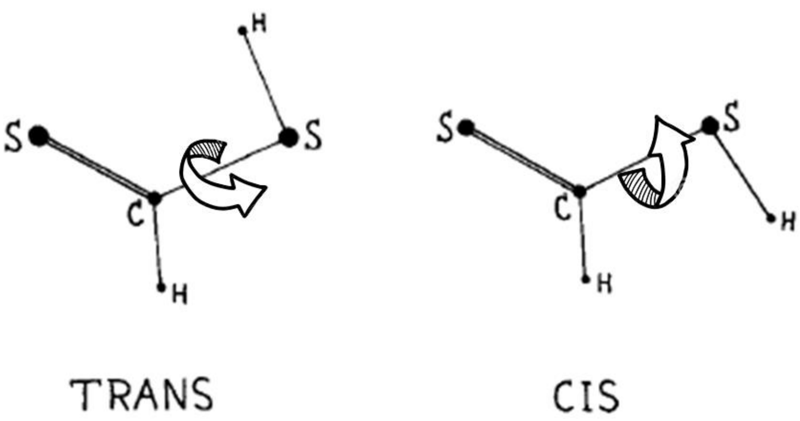
Ab initio calculations



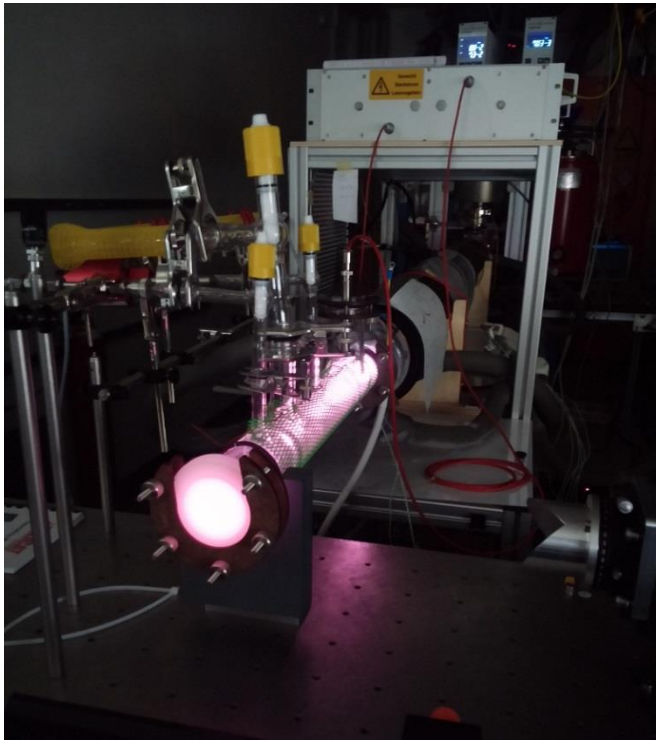
(Prudenzano et al. 2017)

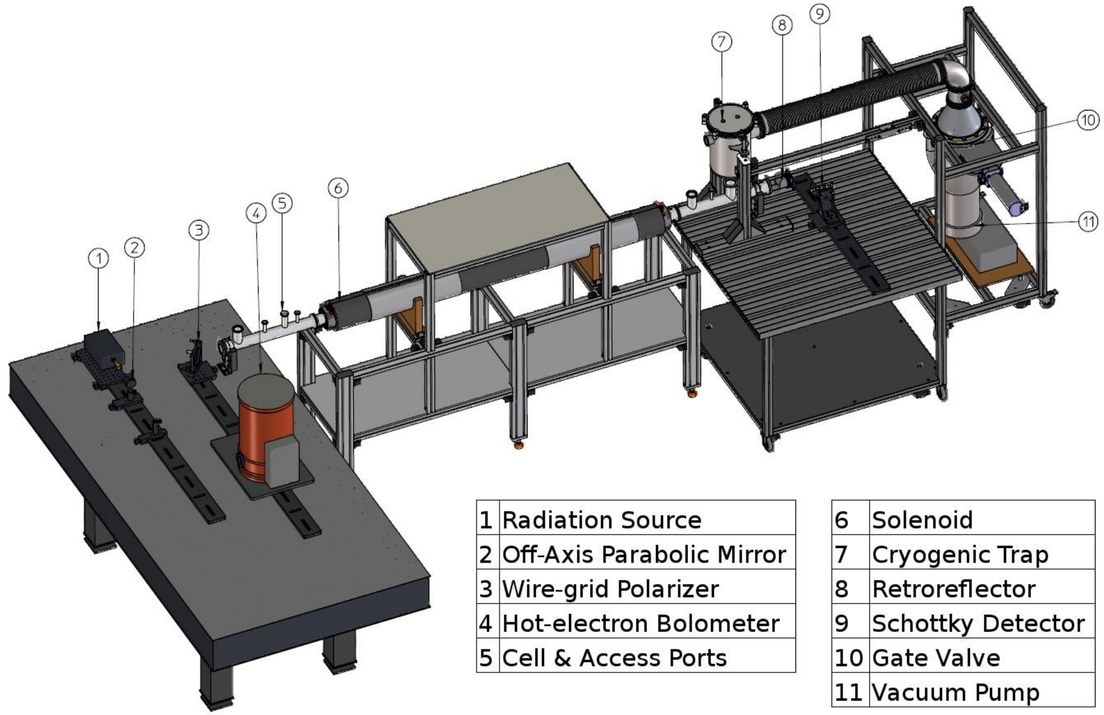
CFOUR software, CCSD(T) method:

-relative energies
-equilibrium geometries
-dipole moments
-rotational barrier
(trans ←→cis)



mm-Wave Spectrometer

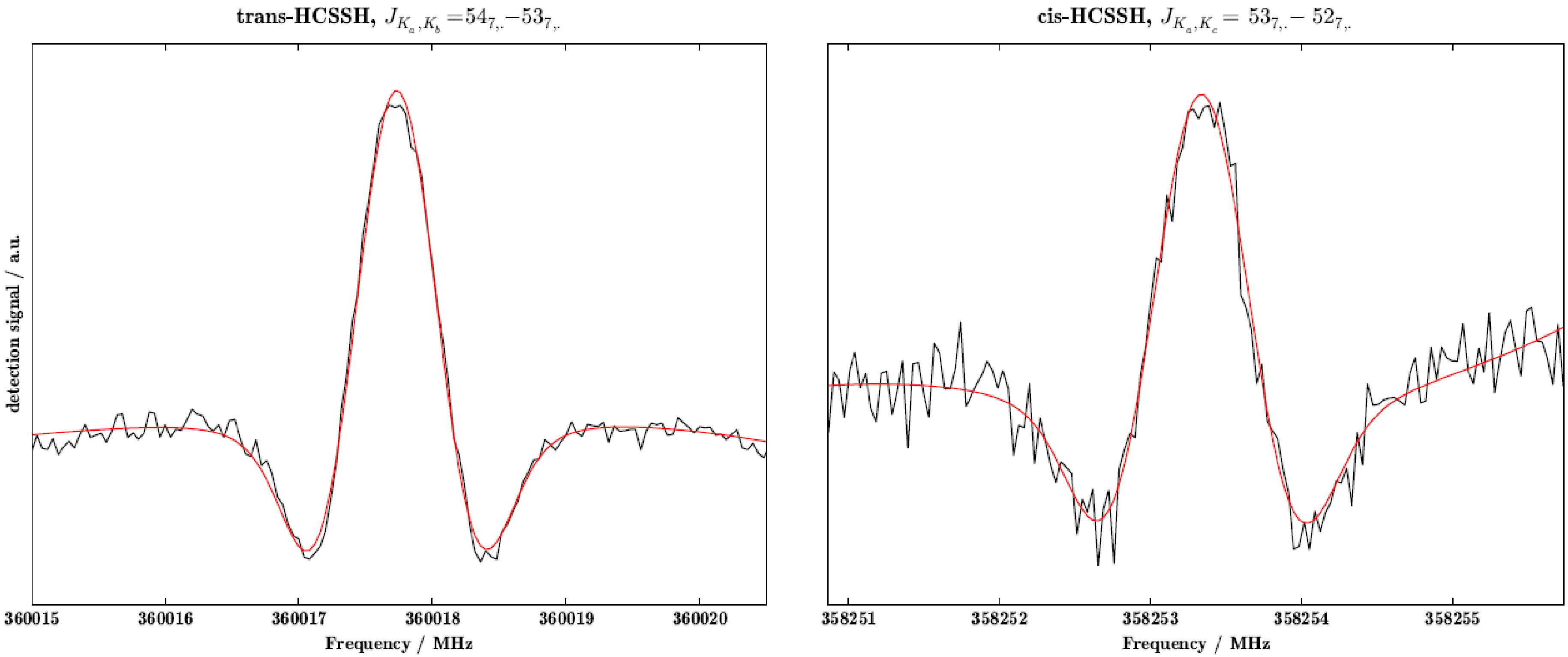




B-enhanced Glow Discharge Cell

- Source Modulation Technique (80 – 1100 GHz)
- Glow discharge of gas mixtures
- Cell T: 120-295 K, $B_{MAX} \approx 250$ Gauss

Results



- H_2 + CS_2 1:1 in Ar (P_{TOT} = 20 - 30 mTorr)
- Line profile fitted with the **proFFit** code(Dore 2003)

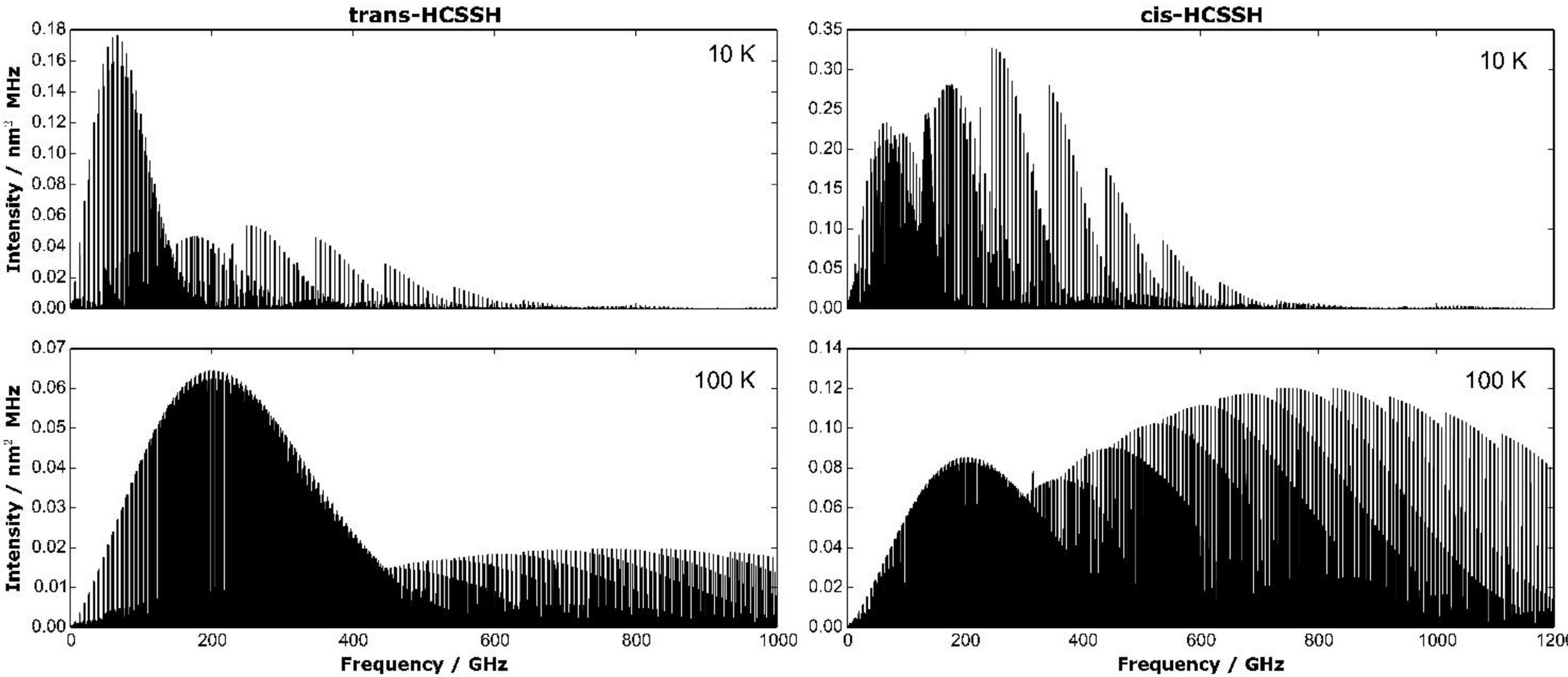
More than 100 experimental lines per conformer, up to K_a=20

Results

Constants	Units	trans-HCSSH[a]	trans-HCSSH[b]	cis-HCSSH[a]	cis-HCSSH[b]
A_0	MHz	49206.11(21)[c]	49227(86)	48572.439(66)	48947(380)
B_0	MHz	3447.53432(37)	3447.5312(89)	3498.74789(67)	3498.719(24)
C_0	MHz	3219.47256(37)	3219.4954(96)	3261.42278(62)	3261.433(30)
D_J	kHz	1.063389(64)	1.10(10)[d]	1.27724(14)	1.02(42)[d]
D_{JK}	MHz	-0.0389438(19)	-0.03905(24)[d]	-0.0470807(33)	-0.0484(12)[d]
D_K	MHz	1.376(33)		1.412(17)	
d_1	Hz	-3.609(38)		4.343(28)	
d_2	kHz	-0.119787(80)		0.14900(20)	
H_{KJ}	Hz	-4.216(15)		-4.109(20)	
H_{JK}	Hz	-0.00573(31)		-0.03601(50)	
H_J	Hz	0.0005714(64)		0.001169(25)	
h_1	Hz	0.0001673(96)		0.000288(38)	
L_{KKJ}	Hz	0.000447(27)			
σ_w		0.936		0.933	
No. of lines		204	25	139	19

[a] This work.
[b] Bak et al. (1978).
[c] Standard error in parentheses in units of the last digits.
[d] Calculated using the Watson's A-reduction for asymmetric top-molecules.

Results



Shocked, sulfur-rich regions with T < 100 K

Estimated uncertainties: 3 kHz @3mm (100 GHz)

12 kHz @1mm (300 GHz)

Conclusions

- New HCSSH accurate measurements
- Improved spectral knowledge towards sub-mm region and complete centrifugal distortion analisys
- Rest frequencies for astronomical searches

Acknowledgements

- Jacob Laas
- Luca Bizzocchi
- Christian Endres
- Valerio Lattanzi
- Michela Giuliano
- Silvia Spezzano

Our director:

- Paola Caselli

THANK YOU
FOR
YOUR ATTENTION