Rotational Spectroscopic Study of Cysteamine

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Sulfur in the Interstellar Space

- Sulfur is the 10th most abundant element in the Universe.
- S-species are sensitive to the changes in the physical conditions and to the chemical age of the studied object.
- S-species have been used as tracers of the protostellar evolution

The main reservoir of Sulphur chemistry in the ISM is an open question the answer to which has baffled astrochemists for decades.

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Methods

Free Jet Absorption Millimeter Wave (FJ-AMMW) spectrometer
Frequency range: **59-118 GHz**
Resolution: 300 kHz
Jet temperature: 6-10K

Molecular Beam Fourier Transform Microwave (MB-FTMW) spectrometer
Frequency range: 6-18 GHz
Resolution: 7 kHz
Jet temperature: 2K

Calabrese, C.; Maris, A.; Evangelisti, L.; Favero, L. B.; Melandri, S.; Caminati, W., J. Phys. Chem. A 2013, 117, 13712−13718.
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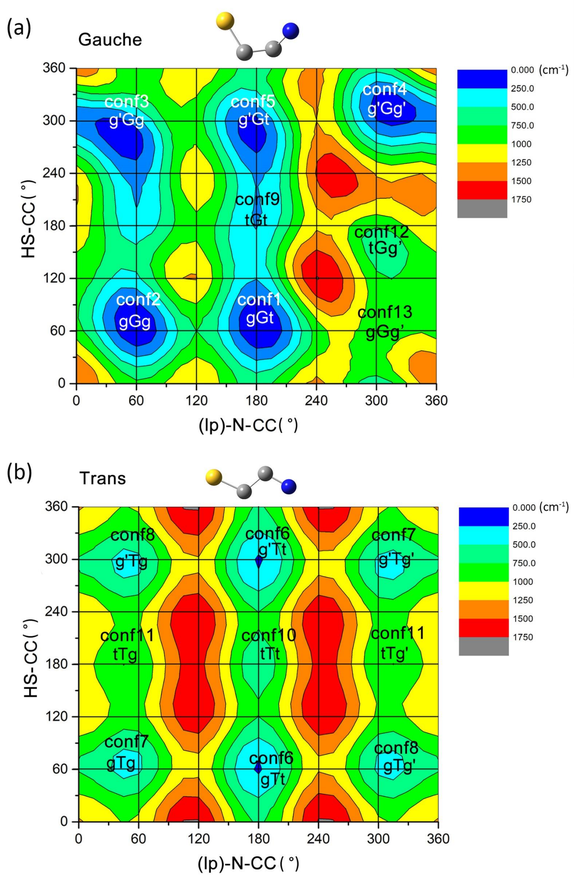
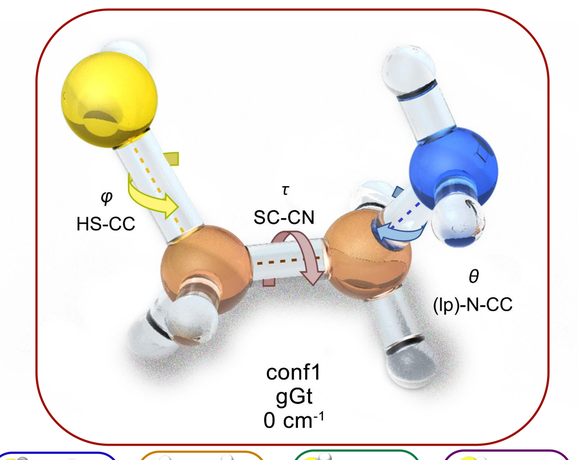
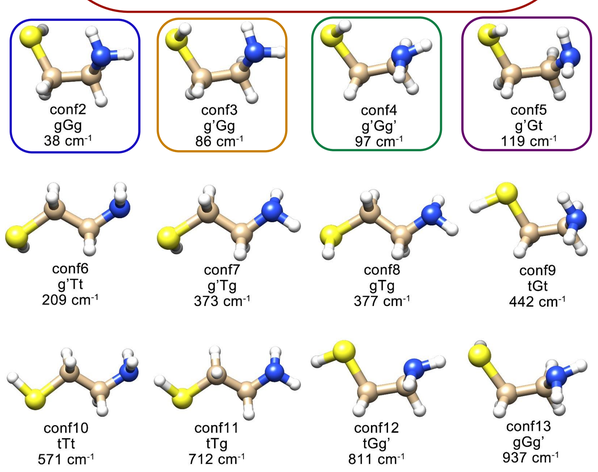
Conformational Space of Cysteamine



2-D potential energy surface of cysteamine with *gauche* and *trans* skeleton.





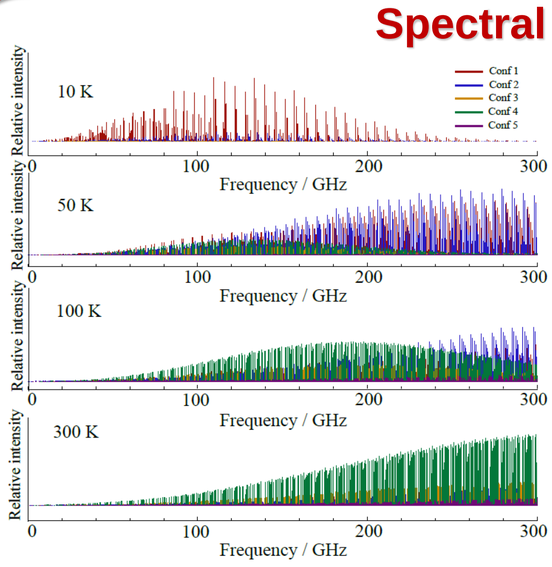
13 stable conformers obtained from the potential surface. All of them have been optimized by Gaussian 16 program at B3LYP-GD3(BJ)/def2-TZVP level

Experimental spectroscopic parameters for all detected conformers of cysteamine

	Conf1	Conf2	Conf3	Conf4	Conf5
A (MHz)	11852.9063(7)[a]	12008.0185(8)	11932.433(2)	12042.9(3)	11944.628(2)
B (MHz)	3310.6341(6)	3363.5781(3)	3394.9980(3)	3552.2284(9)	3292.205(2)
C (MHz)	2866.4712(4)	2898.8592(3)	2877.8302(3)	2881.9906(7)	2827.008(3)
D_J (kHz)	2.13(1)	2.181(5)	2.347(3)	2.201(5)	
D_{JK} (kHz)	-9.95(6)	-10.00(4)	-11.2(1)	-11.83(5)	
D_K (kHz)	39.4(1)	39.6(1)	42.9(2)		
d_1 (kHz)	-0.496(6)	-0.535(3)	-0.616(3)	-0.547(8)	
d_2 (kHz)	-0.030(3)	-0.038(1)	-0.043(3)	-0.025(6)	
$1.5X_{aa}$ (MHz)	-3.873(3)	2.609(3)	2.614(3)	-2.443(8)	-4.77(1)
$0.25(X_{bb}-X_{cc})$ (MHz)	0.481(1)	1.6767(9)	1.703(1)	-0.518(3)	0.422(3)
σ (kHz)	38	40	32	35	6
N	163	304	191	141	16

[a] Standard error in parentheses in the units of the last digit.
[b] Rms deviation of the fit.
[c] Number of transitions in the fit

Spectral Predictions

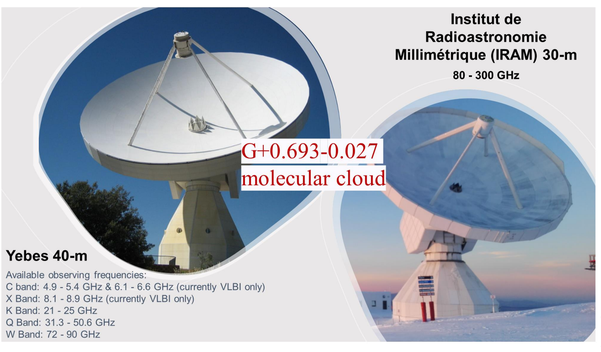


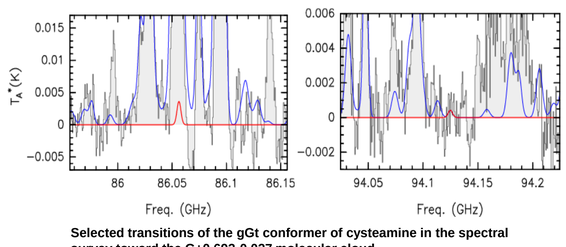
10K
Conf 1&2 dominate at all freq

50 & 100K
Conf 3&4 dominate at low freq
Conf 1&2 dominate at high freq

300K
Conf 3&4 dominate at all freq

Astronomical Survey





Selected transitions of the gGt conformer of cysteamine in the spectral survey toward the G+0.693-0.027 molecular cloud.

Molecular ratios of alcohols and thiols toward the molecular cloud G+0.693-0.027

Molecular family	OH/SH	Reference
CH_3-	23 ± 3	1
$HCO-$ [(a)]	13 ± 4	1
CH_3CH_2-	15 ± 7	1
$NH_2CH_2CH_2-$	>0.8	2 and this work

We have used these transitions to compute the upper limit for the column density of gGt-cysteamine.
In both panels, the grey histogram show the observed spectrum, the blue curve the contribution of all the molecules previously identified in the molecular cloud G+0.693-0.027, and in red the LTE spectrum of the gGt conformer of cysteamine obtained with the upper limit for its column density. Upper limit of the ratio of ethanolamine to cysteamine is calculated to be in 0.8−5.3 range, in agreement with the OH/SH ratios found previously in other molecules.

Conclusions

- Explored the conformational space for cysteamine.
- Determined spectroscopic parameters for the five most stable conformers of cysteamine.
- Predicted rotational spectra of cysteamine at various temperatures.
- Astronomical search for cysteamine towards the G+0.693-0.027 molecular cloud.
- Computed upper limit of the ratio of ethanolamine to cysteamine which are >0.8−5.3, in agreement with the OH/SH ratios found previously in another molecules.