Statistical trends of the GEMS molecular database

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Abstract: The GEMS IRAM 30m Large Program is aimed at estimating the S, C, N, O depletions and the gas ionization degree, X(e), as a function of visual extinction, in a selected set of prototypical star-forming filaments. Using the GEMS observations, we derive the molecular abundances of a selected sample of molecules, first step to the determination of the elemental depletions, and explore the statistical trends of their behaviour. We estimate the physical conditions of 244 points in star-forming filaments of Taurus, Perseus and Orion molecular clouds. We then derive the molecular abundances of 13 species (¹³CO, C¹⁸O, HCO⁺, H¹³CO⁺, HC¹⁸O⁺, H¹³CN, HNC, HCS⁺, CS, SO, ³⁴SO, H₂S and OCS) and explore their behaviour as a function of the gas physical parameters (kinetic temperature, extinction and molecular hydrogen density). We observe strong correlations, particularly between some groups of molecules and between most of the molecular abundances and molecular hydrogen density, which seems to be the main driver of the abundance evolution. This ongoing project provides key information to understand the chemistry involved in the cloud evolution and the star formation process.





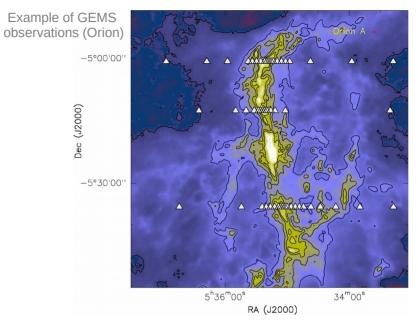
Gas phase Elemental abundances in Molecular cloudS

Fuente et al. (2019), Navarro et al. (2020)

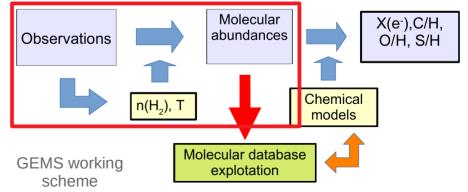
GEMS is an IRAM 30m Large Program aimed at estimating the S, C, N, O depletions and the gas ionization degree, $X(e^{-})$, as a function of visual extinction, in a selected set of prototypical star-forming filaments. The project includes observations towards 305 positions distributed in 27 cuts.

Objective of this work:

The number of observed positions and the homogeneity of the data allows an unprecedented analysis of the statistical trends shown by the molecular abundances in a wide range of physical conditions. This may provide key information to understand the chemical evolution from the diffuse cloud to the prestellar core phase





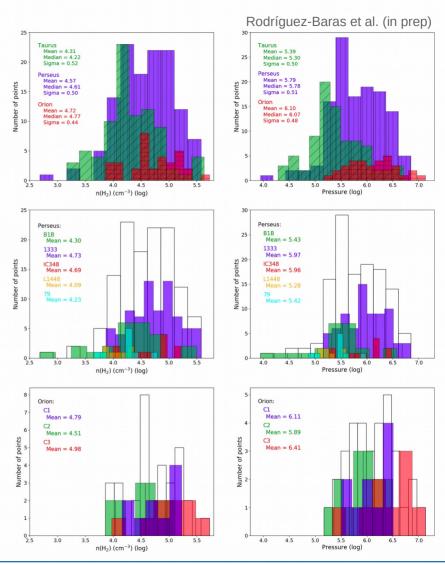




Physical conditions: molecular hydrogen density

A multitransitional analysis of the CS molecule and its isotopologues C³⁴S and ¹³CS is carried out to derive the gas physical conditions, applying the Monte Carlo Markov Chain methodology with a Bayesian inference approach, and using the RADEX code. We derive the molecular hydrogen abundance for 244 positions.

Points belonging to Taurus show the lowest density values, with a peaky distribution. Higher density values and wider distributions are found in Perseus and Orion, related with the feedback of the recent formation of intermediate and high mass stars in the environment.



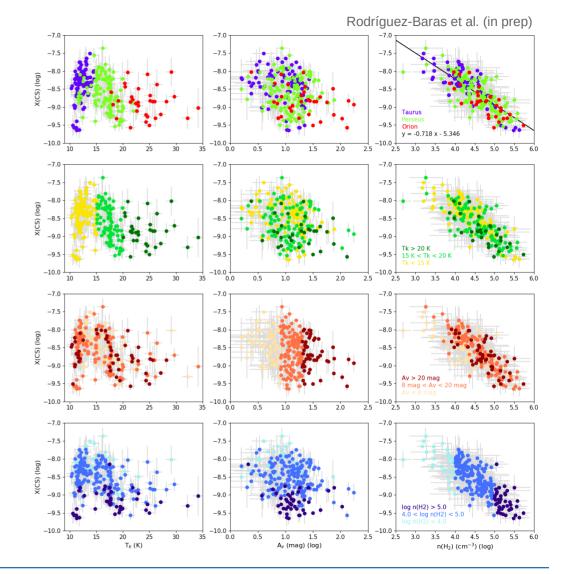
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Molecular abundances

Considering the derived molecular abundances and using the RADEX code, we determine the molecular abundances for the following species: 13 CO, C¹⁸O, HCO⁺, H¹³CO⁺, HC¹⁸O⁺, H¹³CN, HNC, HCS⁺, SO, 34 SO, H₂S and OCS.

We analyze the relation between the molecular abundances and the gas physical parameters (kinetic temperature, extinction and molecular hydrogen density). As an example, these are the results for CS, considering the different clouds and bins of the physical parameters.



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Statistical relations between molecular abundances

	¹³ CO	C18O	HCO+	H ¹³ CO ⁺	HC ¹⁸ O ⁺	H ¹³ CN	HNC	HCS+	CS	so	³⁴ SO	H ₂ S	ocs
¹³ CO -	1.00	0.63	0.43	-0.35	-0.44	-0.33	-0.26	-0.06	-0.14	-0.07	-0.12	0.22	0.11
	(0.0e+00)	(1.3e-25)	(2.9e-11)	(5.5e-06)	(1.4e-05)	(3.4e-04)	(8.3e-05)	(6.1e-01)	(4.5e-02)	(3.2e-01)	(2.2e-01)	(2.9e-03)	(4.6e-01)
C ¹⁸ O -	0.63	1.00	0.17	-0.08	-0.04	-0.06	-0.21	0.36	0.09	0.23	0.07	0.26	0.03
	(1.3e-25)	(0.0e+00)	(6.9e-03)	(3.1e-01)	(6.9e-01)	(4.9e-01)	(1.3e-03)	(5.9e-04)	(1.9e-01)	(7.2e-04)	(4.9e-01)	(2.3e-04)	(8.3e-01)
HCO+ -	0.43	0.17	1.00	0.11	0.04	0.15	0.47	-0.21	0.37	0.31	0.21	0.67	0.38
	(2.9e-11)	(6.9e-03)	(0.0e+00)	(1.4e-01)	(6.6e-01)	(9.5e-02)	(1.9e-14)	(4.7e-02)	(2.2e-09)	(3.1e-06)	(3.0e-02)	(5.3e-27)	(5.8e-03)
H ¹³ CO ⁺ -	-0.35	-0.08	0.11	1.00	0.93	0.84	0.74	0.46	0.60	0.64	0.56	0.48	0.20
	(5.5e-06)	(3.1e-01)	(1.4e-01)	(0.0e+00)	(8.8e-46)	(1.9e-33)	(7.1e-34)	(7.8e-06)	(1.5e-19)	(1.5e-21)	(4.6e-10)	(2.3e-11)	(1.6e-01)
HC ¹⁸ O ⁺ -	-0.44 (1.4e-05)	-0.04 (6.9e-01)	0.04 (6.6e-01)	0.93 (8.8e-46)	1.00 (0.0e+00)	0.83 (1.1e-24)		0.55 (5.0e-07)	0.74 (7.3e-19)		0.58 (2.3e-08)	0.45 (2.3e-06)	0.14 (3.6e-01)
H ¹³ CN -	-0.33	-0.06	0.15	0.84	0.83	1.00	0.78	0.52	0.81	0.56	0.50	0.57	0.16
	(3.4e-04)	(4.9e-01)	(9.5e-02)	(1.9e-33)	(1.1e-24)	(0.0e+00)	(9.0e-27)	(1.7e-06)	(1.0e-29)	(1.1e-11)	(5.9e-07)	(1.4e-11)	(3.4e-01)
HNC -	-0.26	-0.21	0.47	0.74	0.57	0.78	1.00	0.20	0.57	0.48	0.38	0.57	0.19
	(8.3e-05)	(1.3e-03)	(1.9e-14)	(7.1e-34)	(2.0e-10)	(9.0e-27)	(0.0e+00)	(6.9e-02)	(3.4e-22)	(5.2e-14)	(6.8e-05)	(8.3e-19)	(1.7e-01)
HCS ⁺ -	-0.06	0.36	-0.21	0.46	0.55	0.52	0.20	1.00	0.48	0.29	0.17	0.09	-0.08
	(6.1e-01)	(5.9e-04)	(4.7e-02)	(7.8e-06)	(5.0e-07)	(1.7e-06)	(6.9e-02)	(0.0e+00)	(2.6e-06)	(9.4e-03)	(1.8e-01)	(4.0e-01)	(6.6e-01)
CS -	-0.14	0.09	0.37	0.60	0.74	0.81	0.57	0.48	1.00	0.65	0.60	0.71	0.36
	(4.5e-02)	(1.9e-01)	(2.2e-09)	(1.5e-19)	(7.3e-19)	(1.0e-29)	(3.4e-22)	(2.6e-06)	(0.0e+00)	(2.5e-27)	(1.2e-11)	(2.7e-31)	(1.0e-02)
SO -	-0.07 (3.2e-01)	0.23 (7.2e-04)	0.31 (3.1e-06)	0.64 (1.5e-21)			0.48 (5.2e-14)	0.29 (9.4e-03)	0.65 (2.5e-27)	1.00 (0.0e+00)	0.92 (2.0e-45)	0.73 (4.7e-32)	0.72 (2.2e-08)
³⁴ SO -	-0.12 (2.2e-01)	0.07 (4.9e-01)	0.21 (3.0e-02)	0.56 (4.6e-10)		0.50 (5.9e-07)	0.38 (6.8e-05)	0.17 (1.8e-01)	0.60 (1.2e-11)	0.92 (2.0e-45)	1.00 (0.0e+00)		0.72 (2.4e-08)
H₂S -	0.22	0.26	0.67	0.48	0.45	0.57	0.57	0.09	0.71	0.73	0.63	1.00	0.50
	(2.9e-03)	(2.3e-04)	(5.3e-27)	(2.3e-11)	(2.3e-06)	(1.4e-11)	(8.3e-19)	(4.0e-01)	(2.7e-31)	(4.7e-32)	(2.4e-12)	(0.0e+00)	(1.9e-04)
OCS -	0.11	0.03	0.38	0.20	0.14	0.16	0.19	-0.08	0.36	0.72	0.72	0.50	1.00
	(4.6e-01)	(8.3e-01)	(5.8e-03)	(1.6e-01)	(3.6e-01)	(3.4e-01)	(1.7e-01)	(6.6e-01)	(1.0e-02)	(2.2e-08)	(2.4e-08)	(1.9e-04)	(0.0e+00)

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In order to assess the degree of correlation between parameters, we compute the Pearson, Spearman and Kendall correlation coefficients.

Pearson coefficients reveal strong linear correlations between groups of molecules:

- H¹³CO⁺, HC¹⁸O⁺, H¹³CN, HNC and CS, possibly related to depletion on the grain surfaces and variations in the gas ionization degree.
- Sulfuratted species, i. e. CS, SO, ³⁴SO, H₂ S and OCS, which may be caused by the decrease of the atomic S abundance in the gas.

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Statistical relations with physical parameters

Most of the molecules show a strong linear anticorrelation with molecular hydrogen density, spanning over around three orders of magnitude. It seems to be the main driver of abundance evolution.

The correlation with density is always stronger for Taurus. Perseus and Orion recover strong anticorrelations with density for higher extinctions, i.e. in the inner layers of the clouds.

We consider that molecular depletion on the grain surfaces and the decrease of cosmic rays flux with density are the main causes of this behaviour.

This on-going analysis provides key information to understand the chemistry involved in the cloud evolution and the star formation.

		T_k	T _k Spearman	T _k Kendall	A _V Pearson	A _V Spearman	A _V Kendall	n(H ₂) Pearson	n(H ₂) Spearman	n(H ₂) Kendall		
۱.	¹³ CO -	0.57 (2.8e-20)	0.67 (1.4e-30)	0.51 (6.7e-29)	-0.27 (4.3e-05)	-0.30 (7.7e-06)	-0.21 (5.1e-06)	0.11 (1.1e-01)	0.14 (3.4e-02)	0.10 (2.9e-02)		- 1.0
	C ¹⁸ O -	0.15 (2.4e-02)	0.21 (8.2e-04)	0.15 (5.9e-04)	-0.17 (6.8e-03)	-0.13 (4.6e-02)	-0.08 (5.5e-02)	0.06 (3.7e-01)	0.09 (1.7e-01)	0.07 (1.2e-01)		
	HCO+ -	0.46 (3.7e-14)	0.53 (5.7e-19)	0.37 (1.1e-17)	-0.17 (8.1e-03)	-0.13 (4.6e-02)	-0.09 (3.6e-02)	-0.48 (1.6e-15)	-0.39 (3.0e-10)	-0.27 (3.1e-10)		
	H ¹³ CO+ -	-0.44 (3.8e-10)	-0.44 (3.5e-10)	-0.30 (1.5e-09)	0.14 (5.8e-02)	0.28 (1.5e-04)	0.19 (1.1e-04)	-0.54 (1.6e-15)	-0.54 (2.3e-15)	-0.39 (1.8e-15)		
	HC ¹⁸ O ⁺ -	-0.51 (2.2e-08)	-0.47 (3.9e-07)	-0.33 (5.6e-07)	-0.20 (4.3e-02)	-0.06 (5.6e-01)	-0.04 (5.2e-01)	-0.72 (2.7e-18)	-0.71 (1.6e-17)	-0.53 (1.4e-15)		- 0.5
	H ¹³ CN -	-0.39 (8.7e-06)	-0.35 (7.2e-05)	-0.24 (7.1e-05)	0.02 (8.5e-01)	0.13 (1.5e-01)	0.09 (1.6e-01)	-0.84 (2.6e-34)	-0.84 (1.9e-34)	-0.65 (5.6e-27)		
	HNC -	-0.19 (4.1e-03)	-0.20 (1.9e-03)	-0.14 (1.8e-03)	0.19 (2.5e-03)	0.28 (1.2e-05)	0.19 (1.3e-05)	-0.54 (3.4e-19)	-0.48 (2.2e-15)	-0.33 (1.5e-14)		
	CS -	-0.34 (6.6e-08)	-0.35 (1.5e-08)	-0.24 (2.2e-08)	-0.26 (4.8e-05)	-0.22 (6.2e-04)	-0.15 (6.6e-04)	-0.79 (1.7e-53)	-0.78 (2.8e-51)	-0.60 (3.4e-43)		
	HCS ⁺ -	-0.42 (5.0e-05)	-0.34 (1.1e-03)	-0.24 (1.2e-03)	-0.35 (9.5e-04)	-0.27 (1.0e-02)	-0.19 (1.1e-02)	-0.25 (1.8e-02)	-0.24 (2.3e-02)	-0.14 (4.7e-02)		
	SO -	-0.19 (4.8e-03)	-0.17 (1.1e-02)	-0.12 (8.0e-03)	0.08 (2.2e-01)	0.14 (3.8e-02)	0.10 (2.6e-02)	-0.43 (2.0e-11)	-0.43 (5.6e-11)	-0.29 (3.7e-10)		- 0.0
	³⁴ SO -	-0.37 (7.6e-05)	-0.28 (3.1e-03)	-0.20 (2.1e-03)	-0.29 (2.4e-03)	-0.16 (9.9e-02)	-0.11 (9.3e-02)	-0.45 (1.1e-06)	-0.47 (4.4e-07)	-0.31 (1.9e-06)		
	H₂S -	0.03 (6.7e-01)	0.08 (2.4e-01)	0.05 (3.0e-01)	-0.07 (3.4e-01)	-0.04 (5.9e-01)	-0.03 (5.4e-01)	-0.71 (6.1e-32)	-0.69 (1.6e-29)	-0.50 (5.2e-26)		
	OCS -	0.13 (3.6e-01)	0.16 (2.6e-01)	0.13 (1.8e-01)	-0.10 (4.9e-01)	-0.07 (6.3e-01)	-0.05 (6.3e-01)	-0.16 (2.5e-01)	-0.20 (1.5e-01)	-0.14 (1.3e-01)		
	¹³ CO/C ¹⁸ O -	0.56 (1.2e-19)	0.64 (1.1e-26)	0.44 (7.1e-22)	-0.19 (5.0e-03)	-0.17 (1.3e-02)	-0.11 (1.2e-02)	0.08 (2.1e-01)	0.16 (2.1e-02)	0.11 (1.4e-02)		
	CS/SO -	-0.23 (7.3e-04)	-0.26 (1.2e-04)	-0.17 (2.5e-04)	-0.37 (2.1e-08)	-0.41 (2.5e-10)	-0.28 (1.0e-09)	-0.46 (1.9e-12)	-0.45 (2.9e-12)	-0.31 (9.4e-12)		0.5
H1	^{.3} CO ⁺ /H ¹³ CN -	0.09 (3.4e-01)	0.14 (1.2e-01)	0.10 (1.1e-01)	-0.14 (1.1e-01)	-0.15 (8.7e-02)	-0.11 (8.3e-02)	0.44 (2.5e-07)	0.44 (4.0e-07)	0.31 (2.6e-07)		
ŀ	H ¹³ CO+/ ¹³ CO -	-0.59 (5.7e-17)	-0.67 (1.4e-22)	-0.47 (1.1e-18)	0.20 (8.9e-03)	0.26 (9.1e-04)	0.18 (6.8e-04)	-0.54 (6.4e-14)	-0.54 (7.0e-14)	-0.38 (2.5e-13)		
F	HC ¹⁸ O ⁺ /C ¹⁸ O -	-0.60 (2.2e-11)	-0.62 (1.0e-12)	-0.45 (8.0e-12)	-0.12 (2.1e-01)	-0.08 (4.0e-01)	-0.05 (4.5e-01)	-0.62 (1.1e-12)	-0.62 (2.0e-12)	-0.44 (3.2e-11)		
H ¹³	CO+/HC ¹⁸ O+ -	0.07 (4.7e-01)	0.06 (5.7e-01)	0.04 (5.1e-01)	0.15 (1.4e-01)	0.10 (3.3e-01)	0.07 (3.1e-01)	-0.39 (3.1e-05)	-0.40 (2.4e-05)	-0.27 (4.4e-05)		
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