Chemistry of star forming regions including deuteration: modeling and observation

Liton Majumdar

Collaborators:

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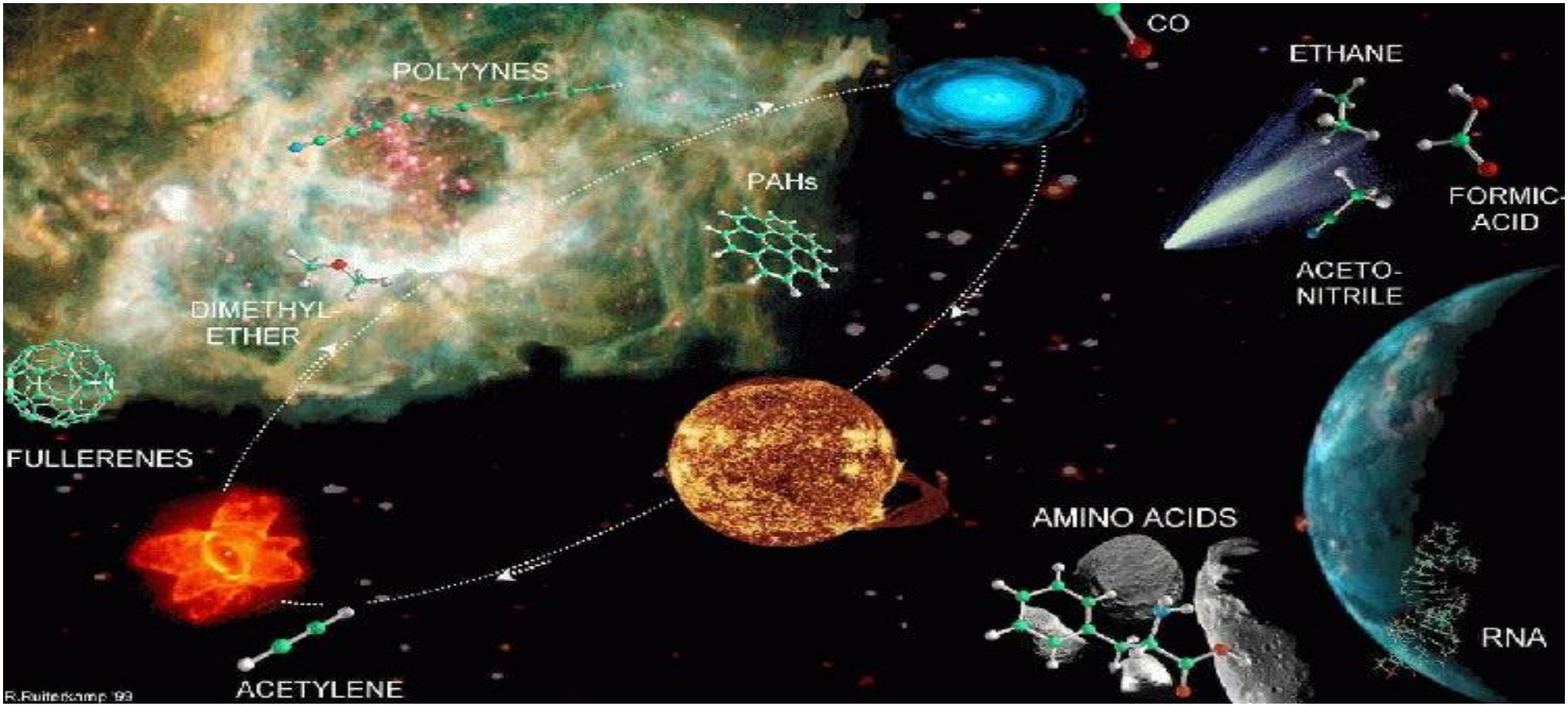
Plan Of My Talk

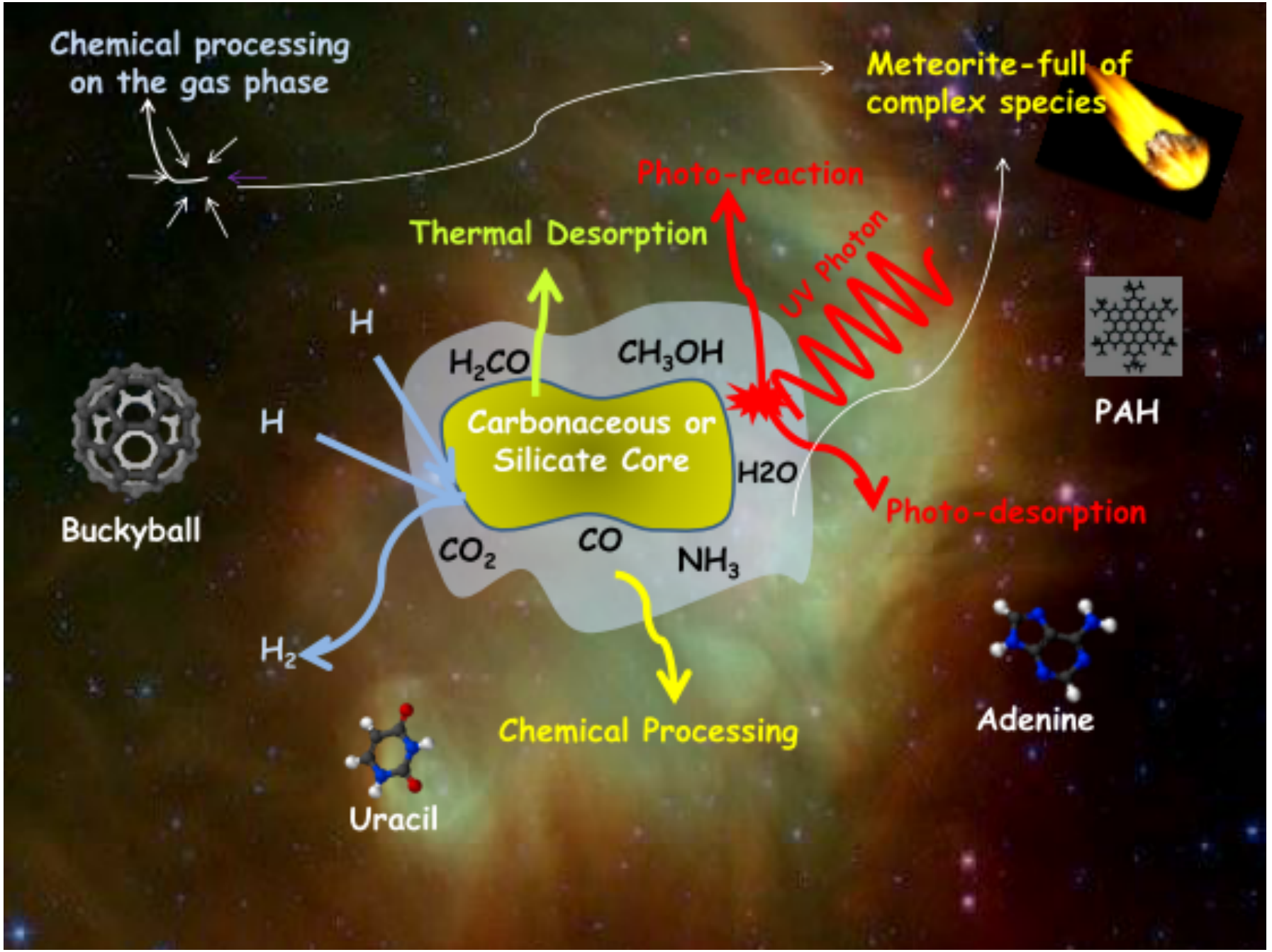
1. Brief introduction of the subject
2. Various tools for studying the chemistry of the ISM
3. Evolving Chemical Composition: (i) Gas phase and (ii) Grain phase including deuteration and spin chemistry for some interstellar species.
4. Different aspects of Astronomical Spectroscopy towards observations
5. Model comparison with the Experiments and Observations
7. Conclusions

Interstellar Medium

ISM is the matter that exists in the space between the star systems in a galaxy. Composition: 99% gas, 1% dust.



Chemical Process involved



Interstellar Cloud

Interstellar cloud is the generic name given to an accumulation of gas, plasma and dust in our galaxy.

Number	Density (cm^{-3})	T(K)	Visual Extinction	Chemistry
Diffuse atomic cloud	10-100	30-100	< 0.1	$f^n_{H2} < 0.1$
Diffuse molecular cloud	100-500	30-100	~ 1	$f^n_{H2} > 1$ CO, CH, CN, C_2, C_3, H_3+, HCO+, OH, C_2H
Translucent cloud	500-1000	15-50	> 1	Chemistry differs due to absence of c^+. conversion of atomic carbon occurs at substantial rate
Dense Molecular cloud	10^4	10	2 - 10	ISRF attenuated so much that rich chemistry occurs, complex molecules may form

The importance of grains and ices for understanding the Chemistry of ISM

A)

atoms

gas-phase

molecules

surface-reactions

grain

Some molecule abundances can only be explained by dust grains or ice surface reactions: e.g., H_2, H_2O methanol, ethanol

B)

molecules

freeze out

ice

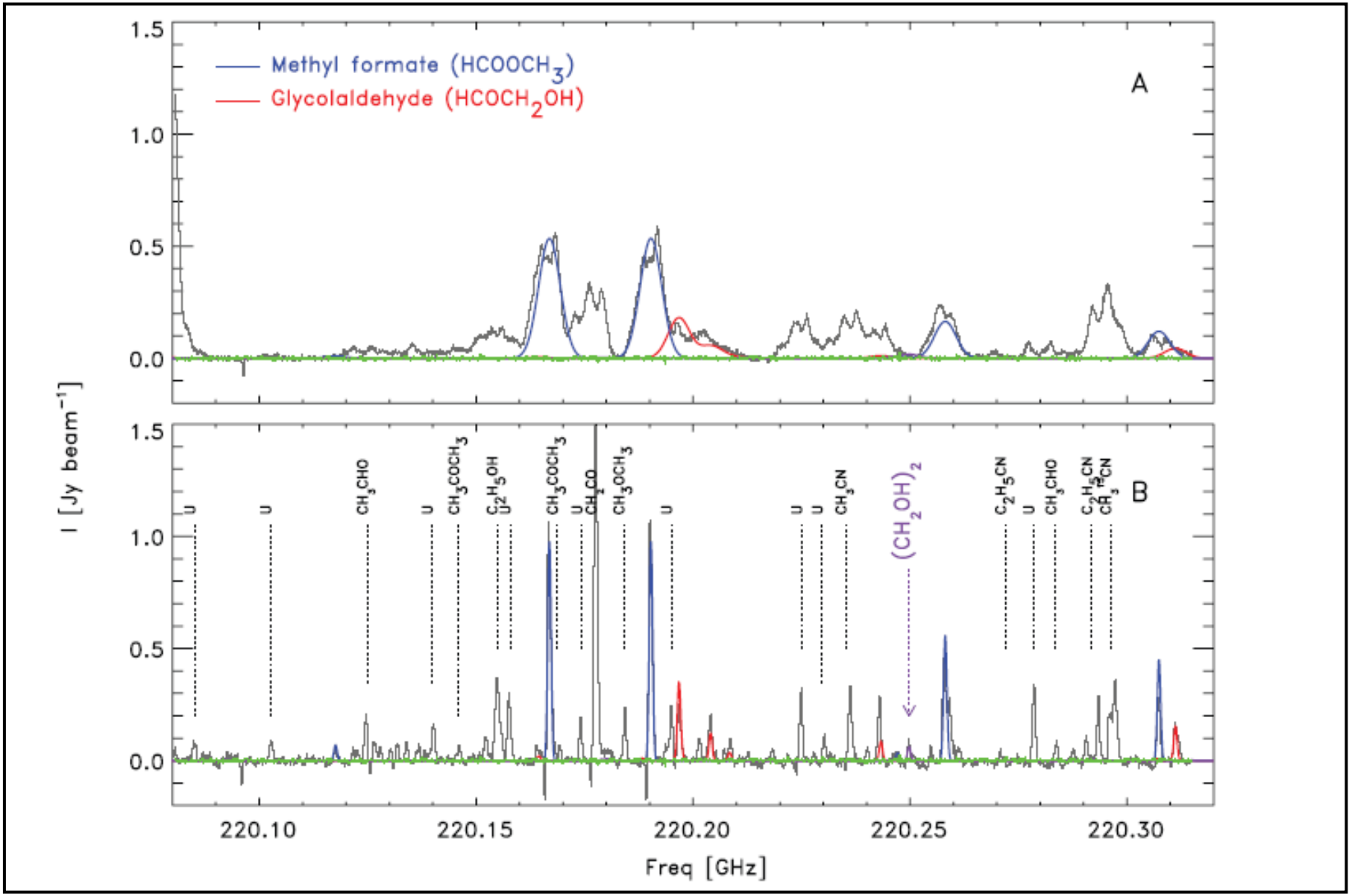
grain

evaporate

Freeze out and evaporation processes controls gas phase abundance hence chemistry significantly during the various evolutionary phases of ISM.

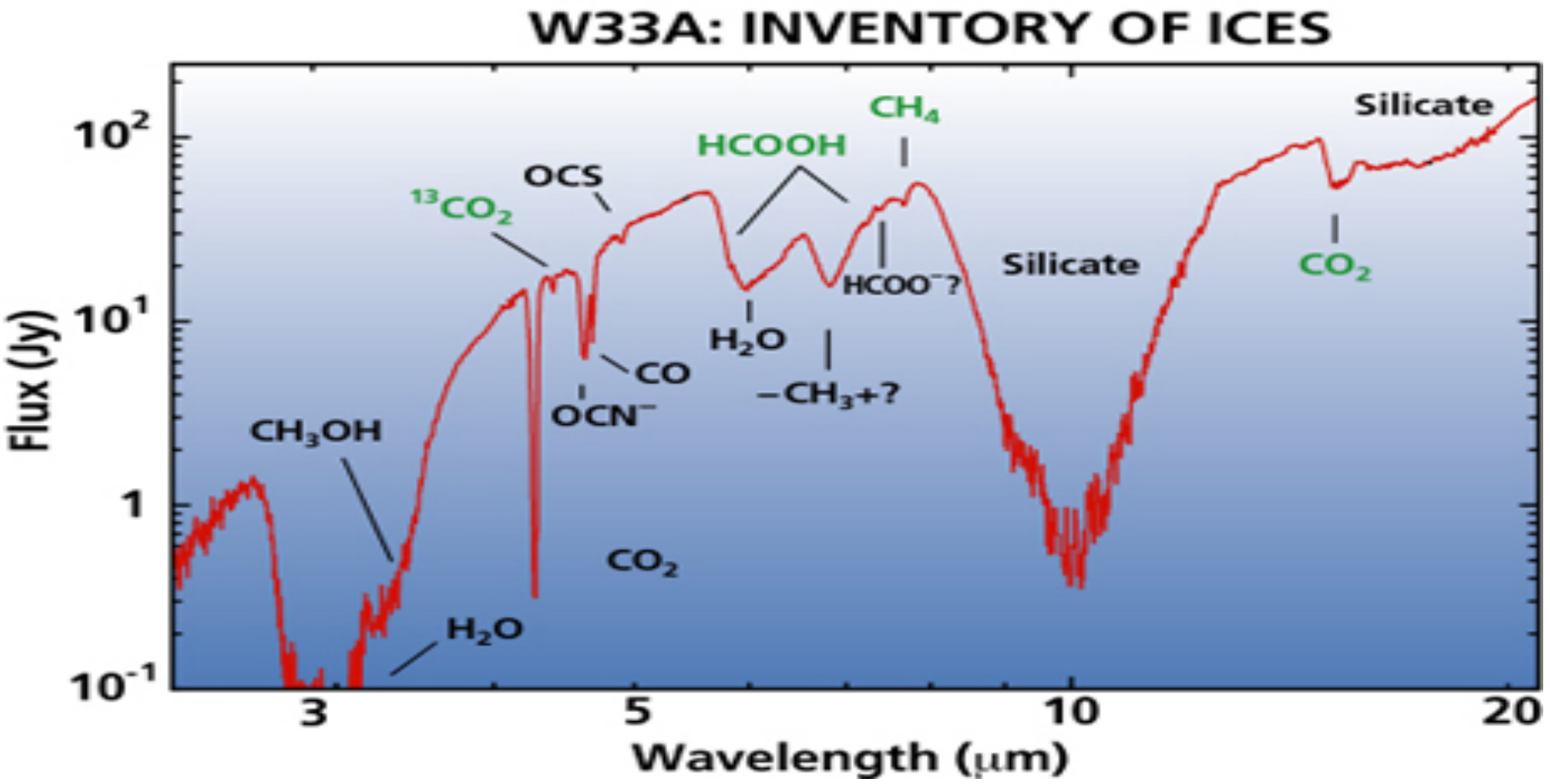
Various Gas phase detections

Detection of simplest Sugar: Glycolaldehyde



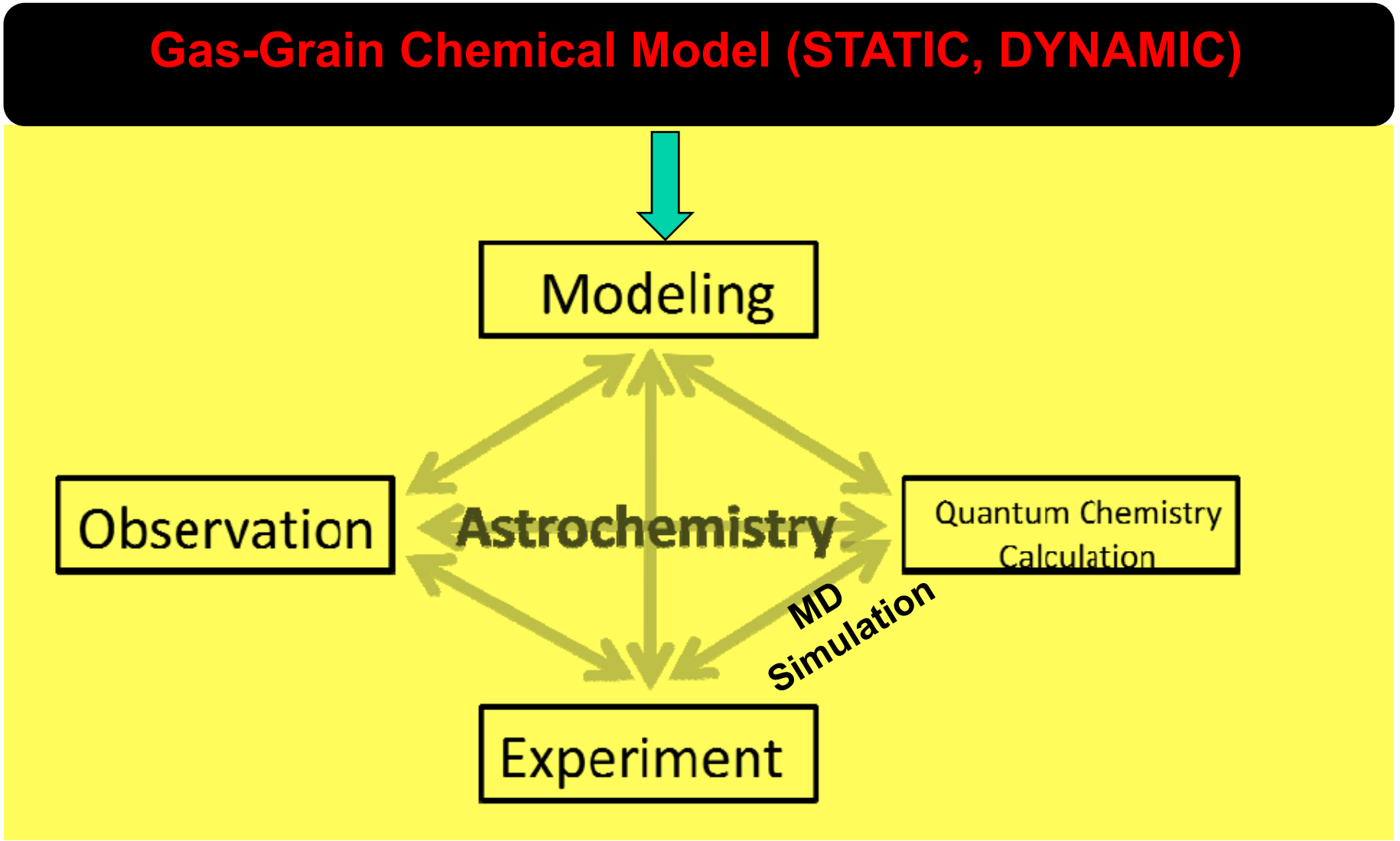
Jorgensen et al., 2012

Observed species on interstellar dusts



Ice is Observed in the Infrared

OUR approaches towards the Astrochemistry



Models used: Previous, Current

- **Previous Model:**

Described in Majumdar et al., (2014a,b), Das & Majumdar et al., (2015, 2014, 2013a,b)

UMIST 2006 database for Gas phase and more reactions from Roberts & Millar (2000), Albertsson et al., (2013), Majumdar et al., (2012).
Hasegawa et al., (1992), Cuppen & Herbst (2007), Garrod et al., (2008), Cazau (2010) for Surface.

- **Current Model with the KIDA Team:**

NAUTILUS gas-grain chemical code.

KIDA 2014 network (Wakelam et al., 2015) for gas phase.

All the updates and network described in Ruaud et al., (2015) for surface chemistry.

Vastel et al., (2012) basic network for spin state and deuterated chemistry along with the various updates from recent papers followed by grain chemistry.

Chemical modeling for few species

Column density

$$N(A) = n_H x_i R$$

Where,

n_H =total hydrogen number density.

x_i = Abundance of i^{th} species,

R= path length along the line of sight
= $1.6 \times 10^{-21} \times A_v / n_H$

Diffuse Interstellar Bands: A Cosmic Mystery

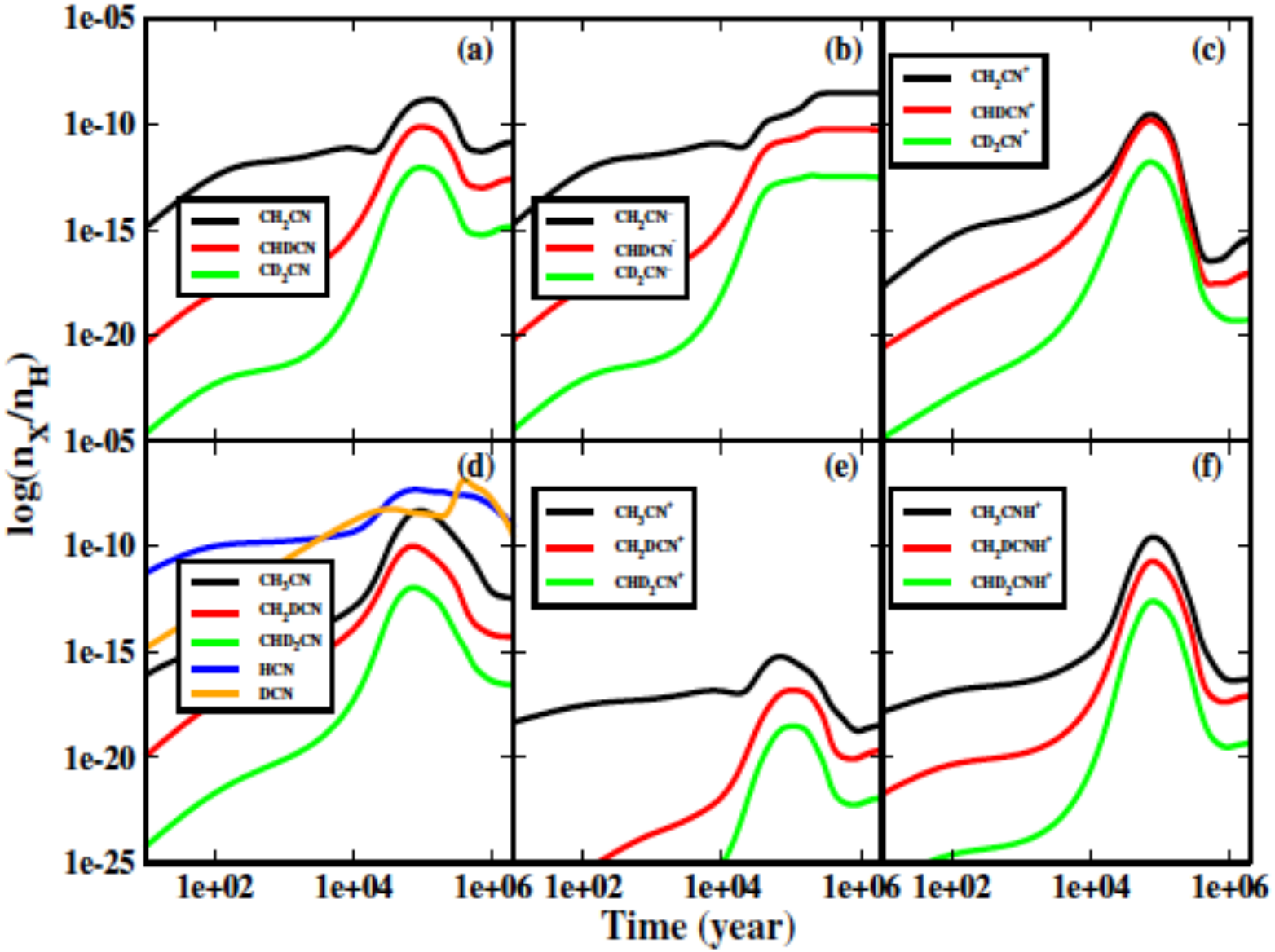
- The DIBs are a series of absorption lines that are observed toward just about every star in the galaxy that has interstellar material in front of it.

- CH_2CN^- might be a carrier of DIBs (Sarre, 2000).

- Possible carrier of the narrow at DIB at 8037± 0.15A^0 (Cordiner and Sarrer, 2007).

- Makes us interested in other forms of CH_2CN^- .

Chemical Modeling for Cyanomethyl anion



Majumdar et al., 2014 (A&A)

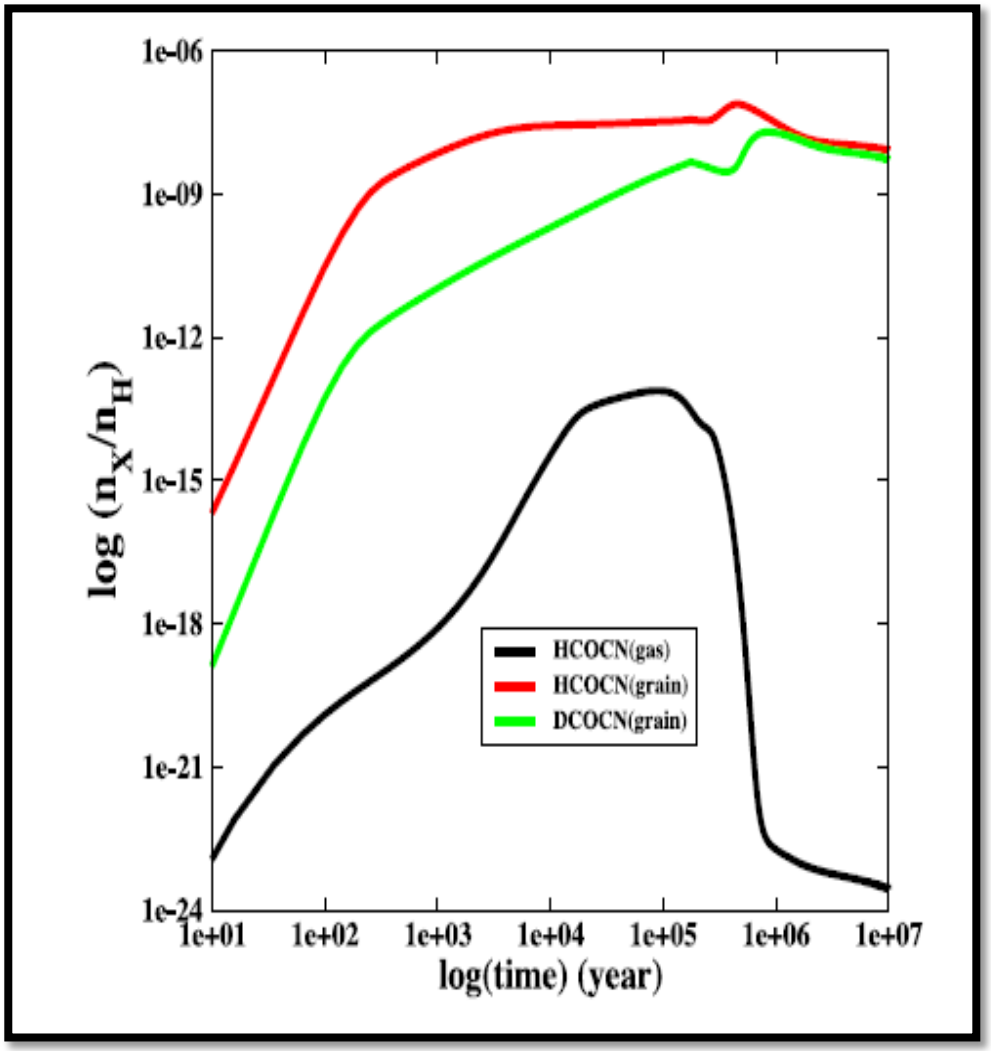
Computed abundances vs Observed abundances

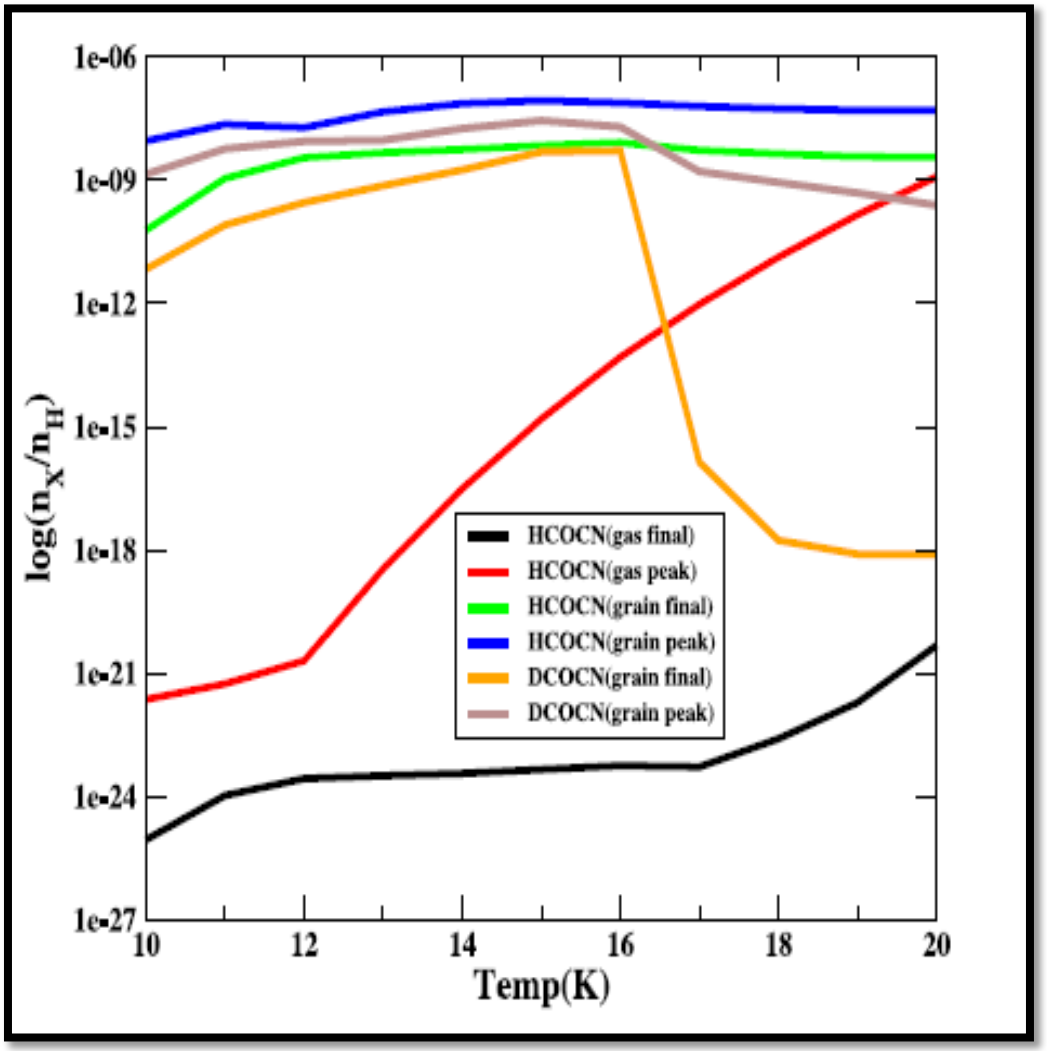
Species	Fractional abundance by observations/other chemical models	Fractional abundance by our model[C]	
		Peak abundance	Abundance after 2×10^6 year
CH_2CN	2.5×10^{-09O}, 4.59×10^{-11W}	1.46×10^{-09}	1.43×10^{-11}
CH_3CN	5.00×10^{-10O}, 6.95×10^{-12W}	5.01×10^{-09}	3.74×10^{-13}
HCN	1.00×10^{-08O}, 2.95×10^{-9W}	4.93×10^{-08}	9.01×10^{-10}
CH_3CN^+	1.02×10^{-18W}	6.24×10^{-16}	3.49×10^{-19}
CH_3CNH^+	2.55×10^{-14W}	2.78×10^{-10}	5.36×10^{-17}
DCN	$2.1–3.7 \times 10^{-10T}$	1.38×10^{-07}	2.69×10^{-10}

Notes. [O] Observation by Ohishi et al. (1992) in TMC-1. [W] Chemical model by Woodall et al. (2007), by considering $n_H = 2 \times 10^4$ cm^{-3}, $T = 10$ K, $A_V = 15$. [T] Observation by Turner (2001) in TMC-1. [C] Our model by considering $n_H = 8984.52$ cm^{-3}, $T = 10$ K, $A_V = 10$.

Majumdar et al., 2014 (A&A)

Cyanoformaldehyde (HCOCN) in the ISM

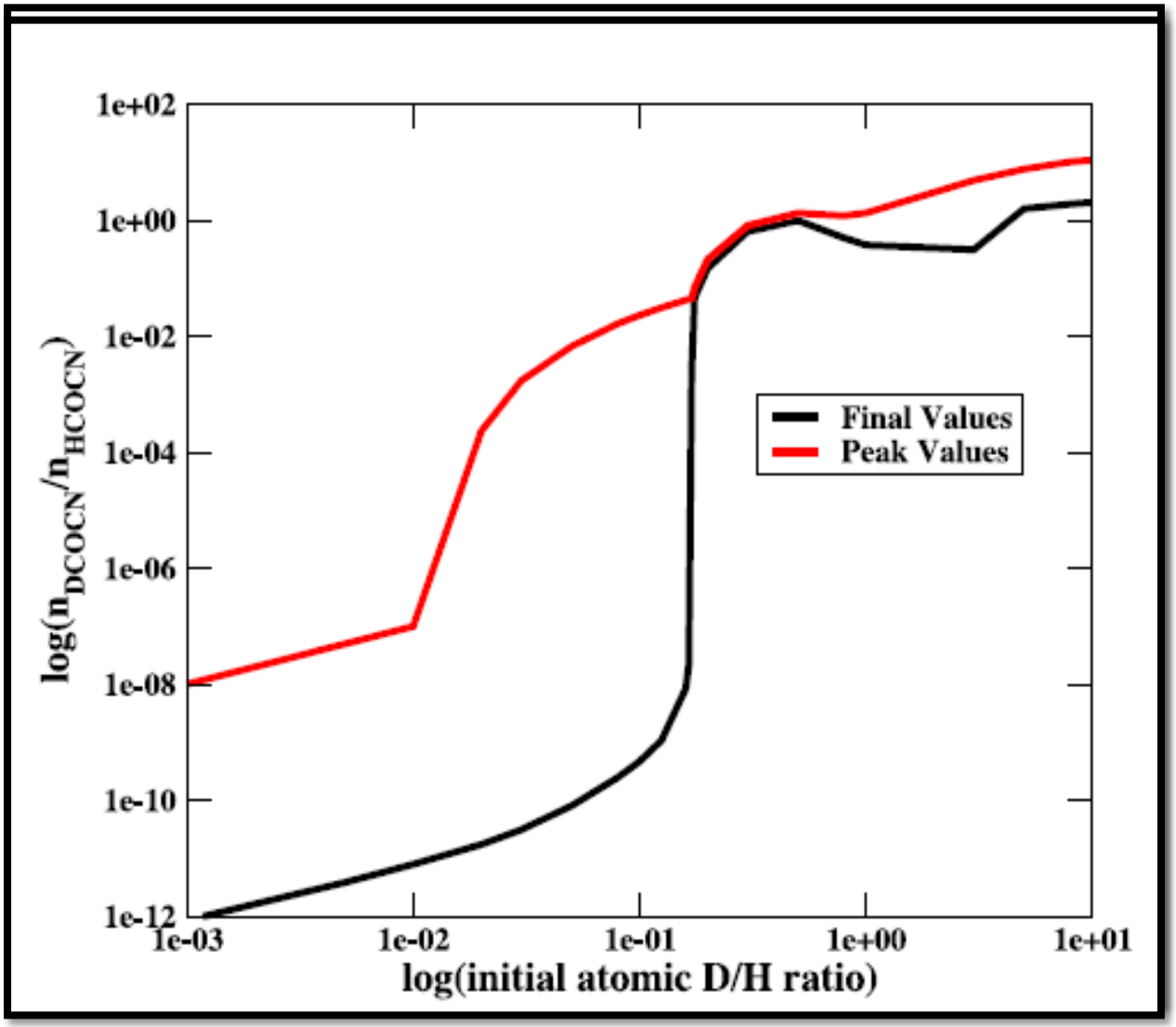




Das, A., Majumdar, L., Chakrabarti, S. K., et al., MNRAS, 2013, 433, 3152

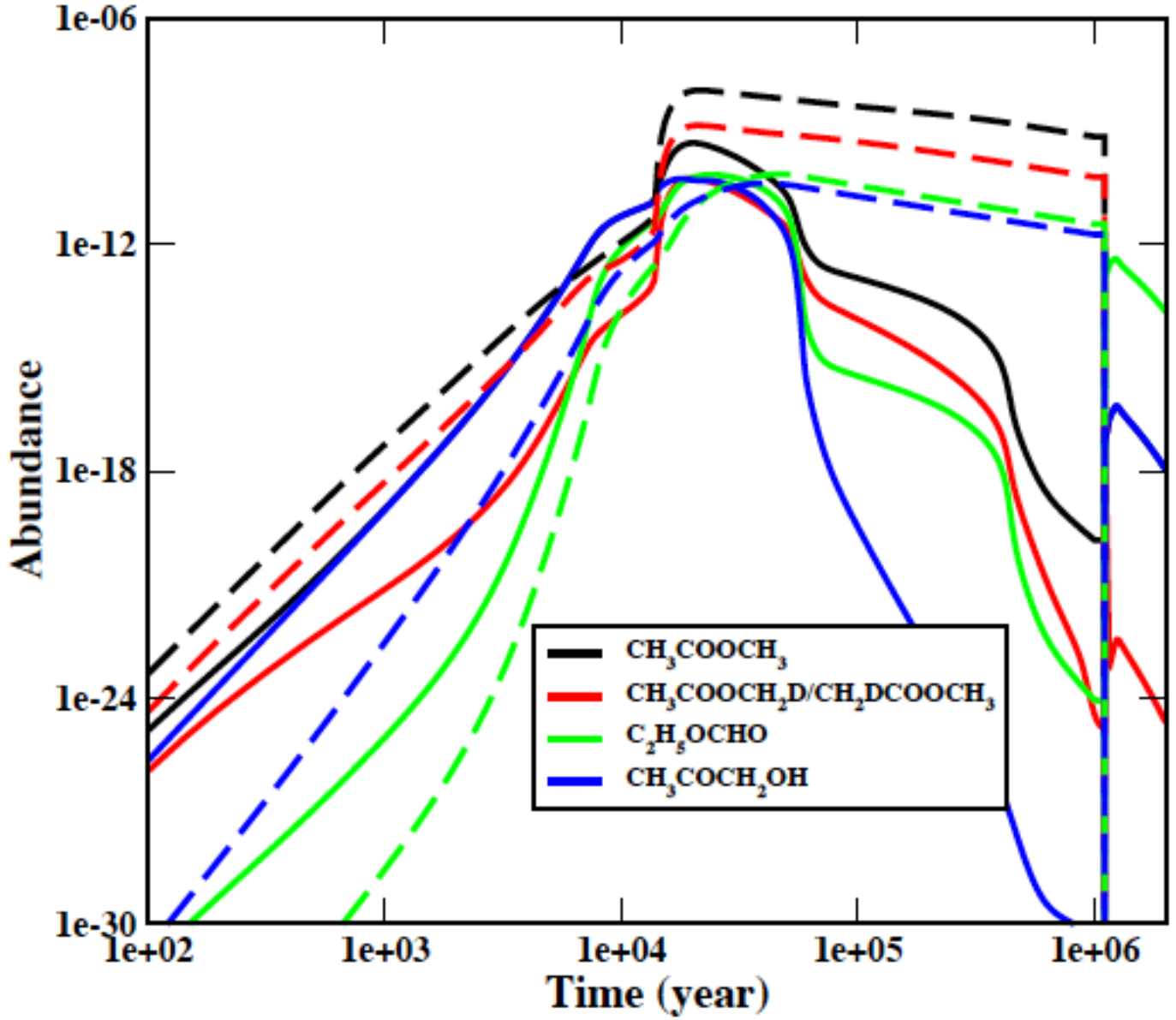
Deuterium Fractionation

❖ Gas phase Cyanoformaldehyde (HCOCN) molecule has recently been suspected towards the Sagittarius B2(N). Our simulation shows that HCOCN and one of its isotopologues (DCOCN) could be traced in the ice phase.



Das, A., Majumdar, L., Chakrabarti, S. K., et al., MNRAS, 2013, 433, 3152

Formation of Methyl Acetate in the ISM



Das, A., Majumdar, L et al., 2015 (ApJ)

Computed Column density vs Observed Column density

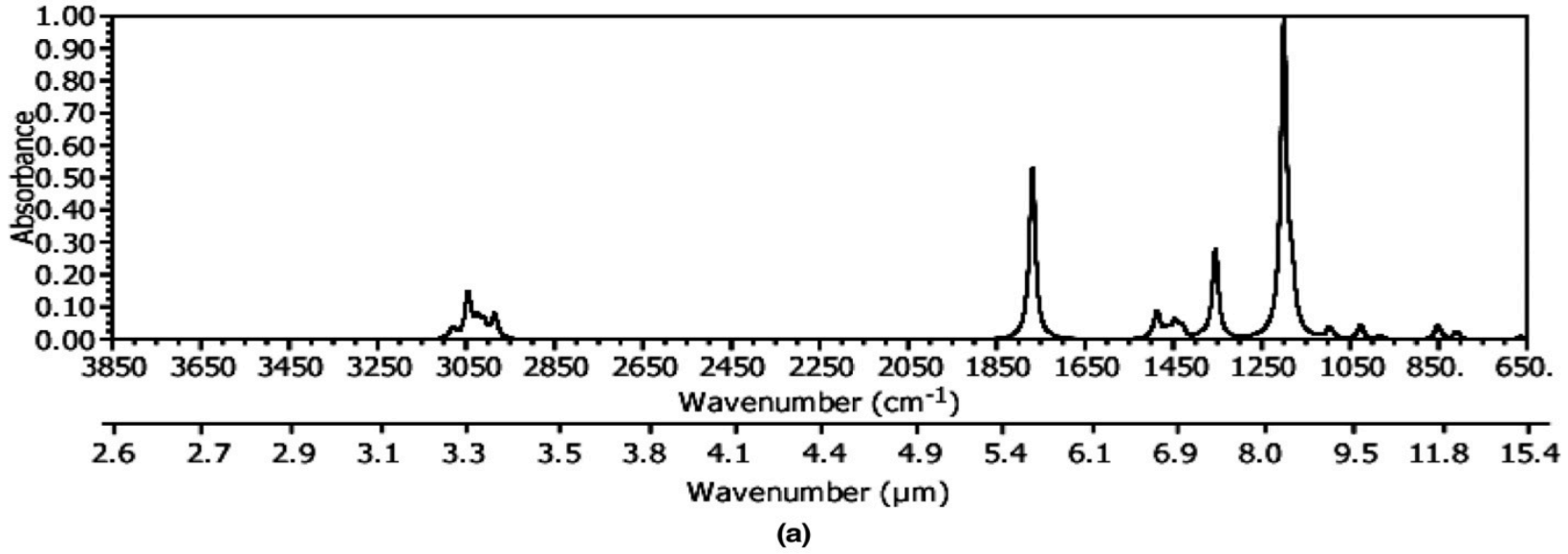
Species	Calculated column density (ice phase peak value) (in cm^{-2})	Calculated column density (gas phase peak value) (in cm^{-2})	Calculated Column density (gas phase final value) (in cm^{-2})	Column density (observation/prediction in gas phase) (in cm^{-2})
CH_3COOCH_3	2.91×10^{15}	1.72×10^{14}	2.58×10^{5}	$(4.2 \pm 0.5) \times 10^{15}$ [a]
$CH_2DCOOCH_3/CH_3COOCH_2D$	3.41×10^{14}	1.46×10^{13}	5.20×10^{-2}	-
C_2H_5OCHO	1.75×10^{13}	8.40×10^{11}	3.95×10^{9}	$(4.5 \pm 1) \times 10^{14}$ [a], 5.4×10^{16} [b]
CH_2COCH_2OH	1.00×10^{13}	4.38×10^{11}	2.59×10^{5}	5.00×10^{12} [c]

[a] Tercero et al. (2013) (in Orion)
[b] Belloche et al. (2009) (in Sgr B2(N))
[c] Apponi et al. (2006) (in Sgr B2(N))

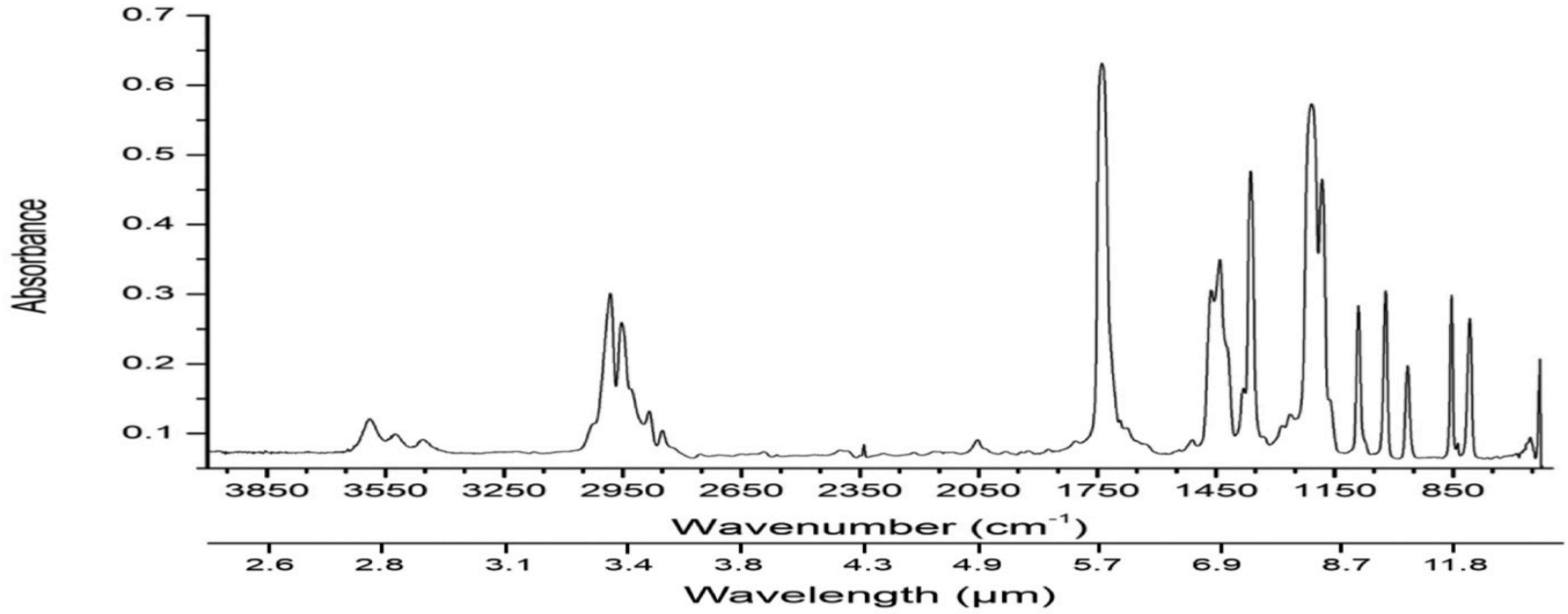
Das, A., Majumdar, L et al., ApJ (2015)

Astronomical Spectroscopy

Methyl Propionate ($CH_3CH_2COOCH_3$) in ICY ASTROCHEMICAL conditions



(a)

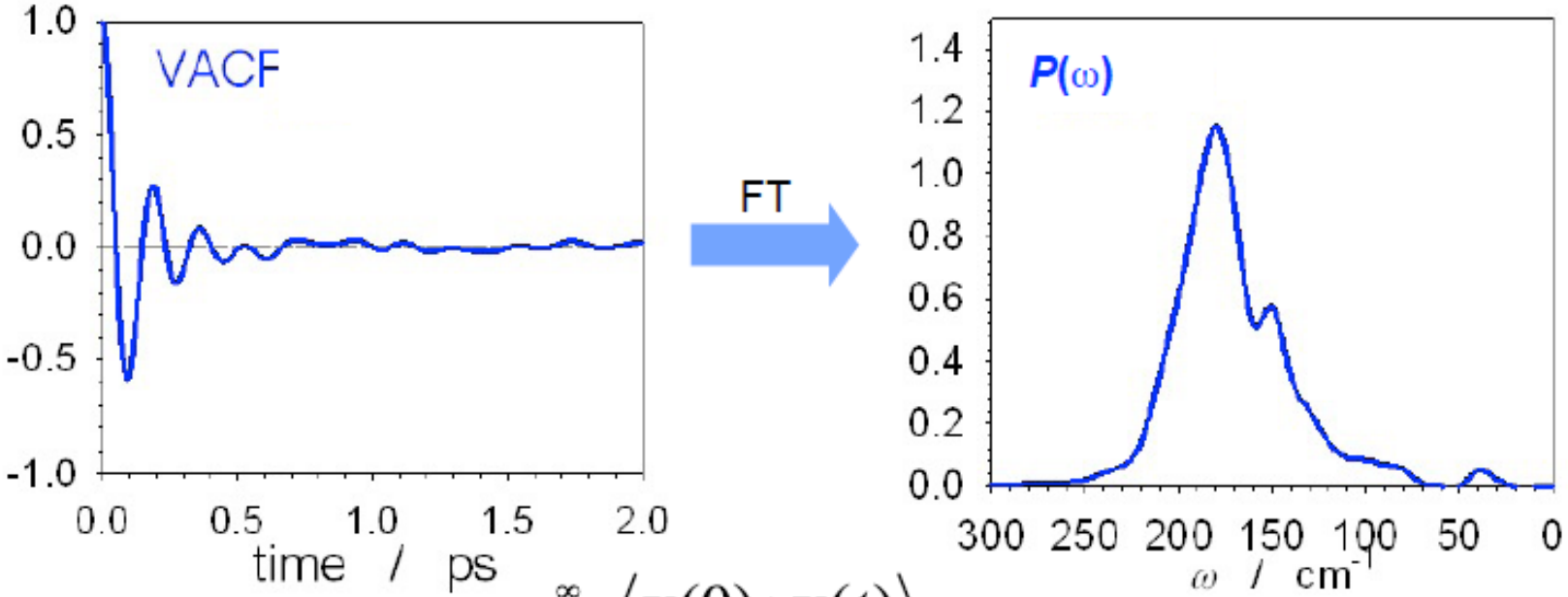


(b)

Sivaraman et al., 2015 (MNRAS)

Molecular Dynamics simulation in the context of Astrochemistry: Physics on Interstellar Dusts

$$\mathrm{VACF} \equiv C_{vv}(t) = \frac{\langle \mathbf{v}(0) \times \mathbf{v}(t) \rangle}{\langle \mathbf{v}(0)^2 \rangle} = \frac{1}{\langle \mathbf{v}(0)^2 \rangle} \int \mathbf{v}(0) \times \mathbf{v}(t)\, d\Gamma$$

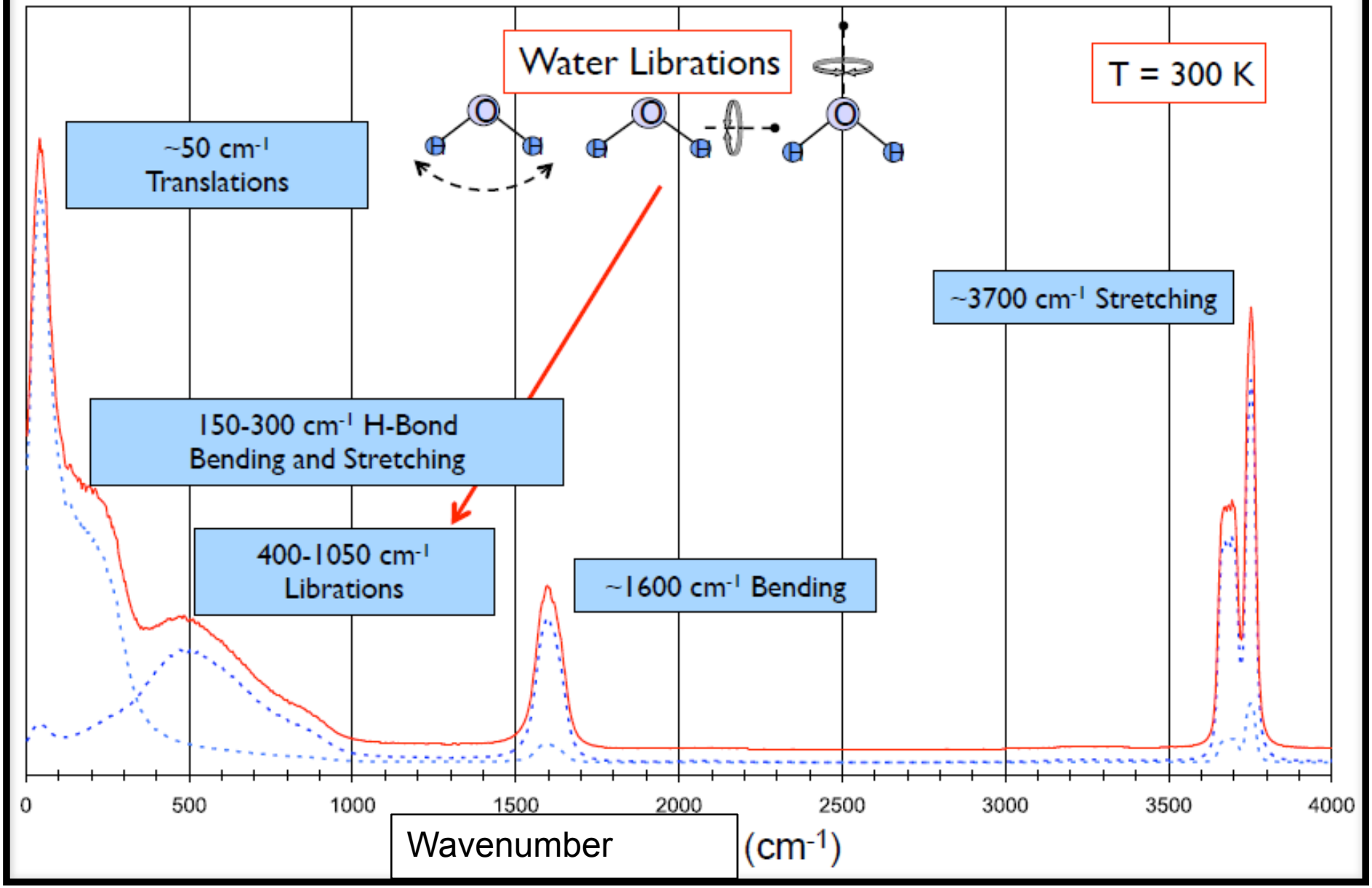


$$P(\omega) = \int_0^{\infty} \frac{\langle \mathbf{v}(0) \times \mathbf{v}(t) \rangle}{\langle \mathbf{v}(0)^2 \rangle} \cos(\omega t)\, dt$$

VACF = velocity autocorrelation function

Majumdar et al., 2015 (In Prep.)

Power Spectra of Water



Majumdar et al., 2015 (In Prep.)

Data required for Astronomical Spectroscopy

Species	Rotational constants	Values in MHz	Experimental values in MHz[a]	Distortional constants	Values in MHz	Experimental values in MHz[a]
HCOCN in gas phase	A	66034.4	67473.54	Δ_J	2.267×10^{-3}	2.266×10^{-3}
	B	4975.9	5010.19	Δ_{JK}	-0.1413	-0.143104
	C	4627.1	4656.498	Δ_K	7.074	8.99
				δ_j	3.933×10^{-4}	3.877×10^{-4}
				δ_k	0.02895	0.034325

[a] Bogey et al., (1988)

Our results are in excellent agreement with the experiment

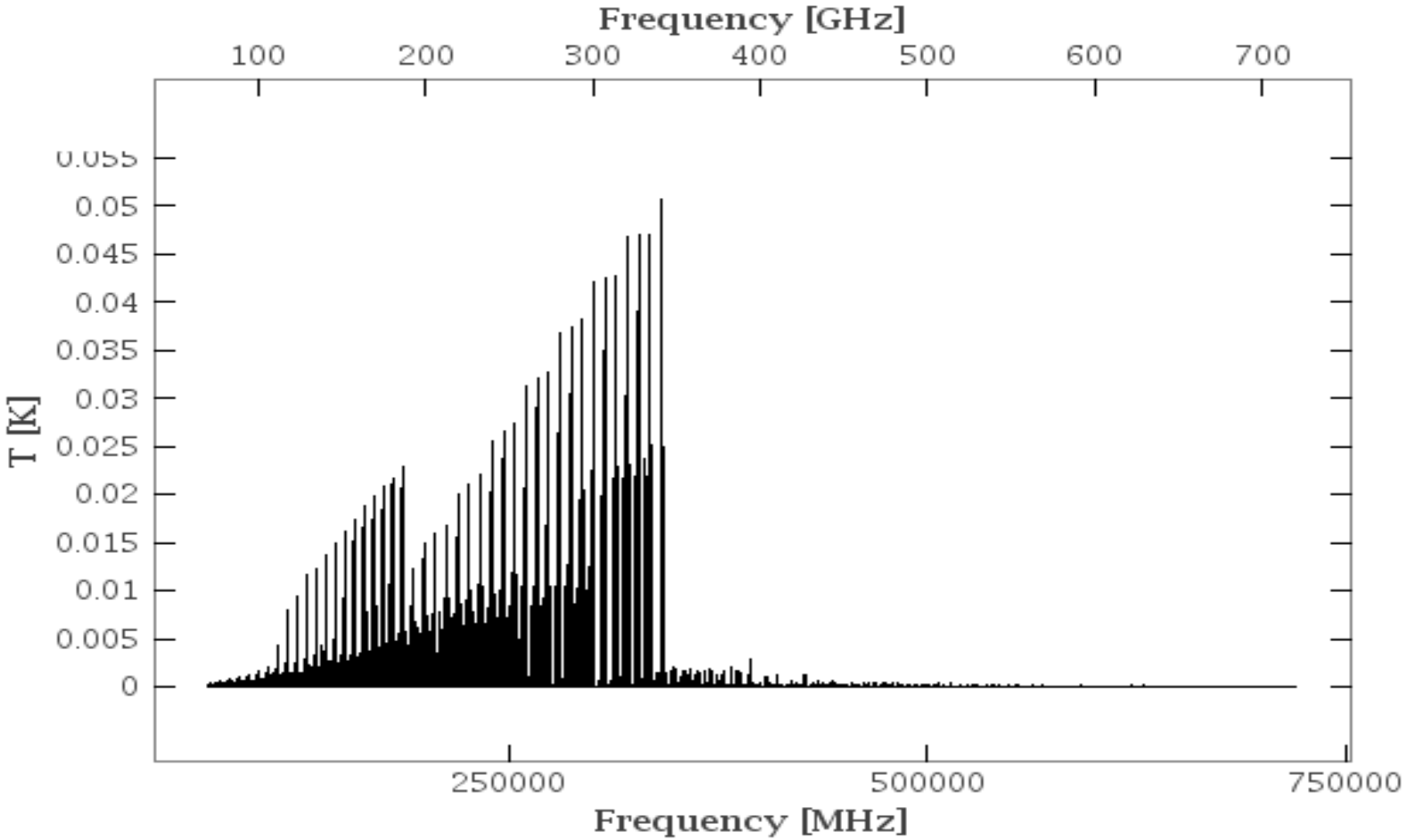
Das, A., Majumdar, L., Chakrabarti, S. K., et al., MNRAS, 433, 3152

Rotational spectrum information for HCOCN molecule in JPL catalog format using SPFIT/SPCAT codes

Frequency[a]	Uncertainty[b]	I[c]	D[d]	E_{lower}[e]	g_{up}[f]	Tag[g]	QnF[h]	Qn_{up}[i]	Qn_{lower}[j]
9602.0577	0.0000	-7.3358	3	-0.0000	3	55001	304	1 0 1 1	0 0 0 1
9603.2441	0.0000	-7.1139	3	-0.0000	5	55001	304	1 0 1 2	0 0 0 1
9605.0238	0.0000	-7.8128	3	-0.0000	1	55001	304	1 0 1 0	0 0 0 1
19204.8519	0.0000	-7.0358	3	0.3203	5	55001	304	2 0 2 2	1 0 1 2
19205.0496	0.0000	-6.9108	3	0.3204	3	55001	304	2 0 2 1	1 0 1 0
19206.0382	0.0000	-6.5586	3	0.3203	5	55001	304	2 0 2 2	1 0 1 1
19206.1230	0.0000	-6.2875	3	0.3203	7	55001	304	2 0 2 3	1 0 1 2
19206.8293	0.0000	-8.2117	3	0.3203	3	55001	304	2 0 2 1	1 0 1 2
19208.0157	0.0000	-7.0357	3	0.3203	3	55001	304	2 0 2 1	1 0 1 1
28807.6502	0.0000	-6.8613	3	0.9610	7	55001	304	3 0 3 3	2 0 2 3
28808.7236	0.0000	-6.1289	3	0.9610	5	55001	304	3 0 3 2	2 0 2 1
28808.9213	0.0000	-5.9582	3	0.9609	7	55001	304	3 0 3 3	2 0 2 2
28808.9684	0.0000	-5.7979	3	0.9610	9	55001	304	3 0 3 4	2 0 2 3
28809.4299	0.0000	-8.4052	3	0.9610	5	55001	304	3 0 3 2	2 0 2 3
28810.7010	0.0000	-6.8613	3	0.9609	5	55001	304	3 0 3 2	2 0 2 2
38410.3229	0.0000	-6.7387	3	1.9219	9	55001	304	4 0 4 4	3 0 3 4
38411.5564	0.0000	-5.6807	3	1.9220	7	55001	304	4 0 4 3	3 0 3 2
38411.6412	0.0000	-5.5626	3	1.9219	9	55001	304	4 0 4 4	3 0 3 3
38411.6711	0.0000	-5.4474	3	1.9219	11	55001	304	4 0 4 5	3 0 3 4
38412.0179	0.0000	-8.5379	3	1.9219	7	55001	304	4 0 4 3	3 0 3 4
38413.3361	0.0000	-6.7387	3	1.9219	7	55001	304	4 0 4 3	3 0 3 3
48012.7951	0.0000	-6.6448	3	3.2032	11	55001	304	5 0 5 5	4 0 4 5

Das, A., Majumdar, L., Chakrabarti, S. K., et al., MNRAS, 433, 3152

Emission Modeling for one of the isomer of Methyl Acetate molecule around ALMA 3 to 9 Band (84-720 GHz)



Das, A., Majumdar, L et al., ApJ (2015)

Why Spin Chemistry is important in chemical modeling

- Pagani et al., (1992, 2009), Flower et al., (2004, 2006a,b), Walmsley et al., (2004) - ortho para spin modifications of H and D bearing species is important due to some reactions are faster with ortho-H_2 than para-H_2 and thus can change the entire chemistry of deuterium fractionation.

- For example- backward reaction of $H_3^+ + HD \rightarrow H_2D^+ + H_2$ is endothermic by 232 K and so could be negligible at low temperature. But if we consider ortho spin state of H_2 and H_2D^+ then the reaction becomes exothermic by 85 K and thus no longer negligible because it slows down the deuterium fractionation.

- Thus it would be necessary to classify the important reactions of ortho, para, meta states of H_2, D_2, H_2^+, D_2^+, H_3^+, H_2D^+, D_2H^+ which are the main species in Deuterium fractionation (Ceccarelli et al., 2014).

- Extend ortho and para chemistry for others- ortho-NH_2^+, para-NH_2^+ etc.

- Nuclear spin conversion on grain.

Very Basic Model for GG Tau A System

Chemistry around GG Tau disk midplane (200 AU):

Observational parameters used in the model: H_2 surface density - 10^{24} cm^{-2}

Dust temperature – 14 K

Grain size- 0.1 Micrometer

High Cosmic Ray regime (10^{-17} s^{-1}) –
Computed Abundance- 2 X 10^{-11} Computed Column density- 2 X10^{-13} cm^{-2}

Low Cosmic Ray regime (10^{-17} s^{-1})-
Computed Abundance- 7 X 10^{-13} Computed Column density- 7 X10^{11} cm^{-2}

Majumdar et al., 2015 (In Pre.)

Conclusions

- We have pointed out that the production of various molecules in the ISM are within the observed limit and could be detected in future.

- How quantum chemical simulation as well as molecular dynamics simulation can be used as a useful tool to explain the physics and chemistry of interstellar species.

- Various aspects of astronomical spectroscopy on interstellar circumstances are discussed.

- Guidelines for the detections of more complex species in the ISM are discussed.

Acknowledgements:

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Thank You