

The excitation of ethynyl in the interstellar medium : A key to understand isotopic fractionation ?

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The case of ethynyl (C_2H)...

C_2H has been discovered in a wide range of astrophysical environments:

- Photodissociation regions
- Pre-stellar cores
- High-mass star forming regions
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This molecule is one of the most abundant hydrocarbon in the ISM

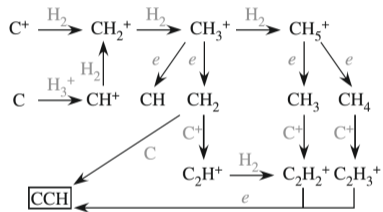


Figure: Formation pathway¹ of C_2H

¹Sakai *et al.*, A&A 512, A31 (2010)

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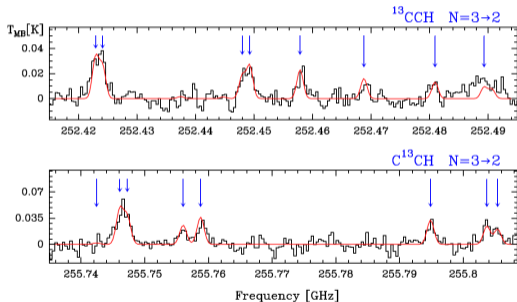
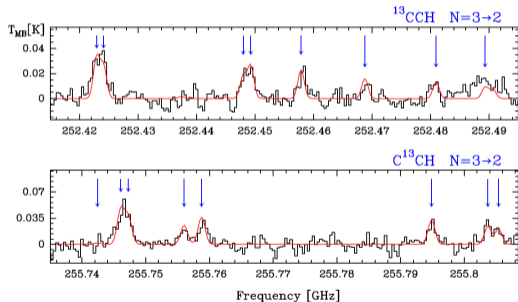


Figure: Detected C_2H isotopologues hyperfine lines of the $N = 3 \rightarrow 2$ rotational transitions¹

Hyperfine resolved spectra show a higher intensity in favor of $C^{13}CH$ lines than ^{13}CCH ones. Two reasons can explain these anomalies:

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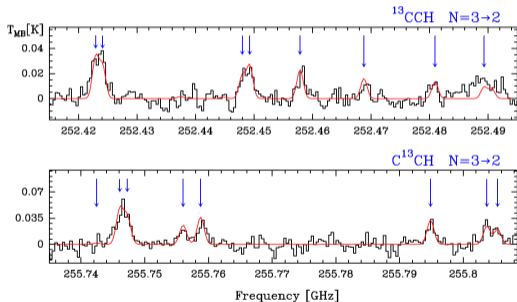


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Hyperfine resolved spectra show a higher intensity in favor of C¹³CH lines than ¹³CCH ones. Two reasons can explain these anomalies:

- Different formation processes
- Different excitation mechanisms

⇒ **Need accurate rate coefficients induced by H₂ in order to interpret observations**

¹Cuadrado *et al.*, A&A 575, A82 (2015)

Obtention of the $^{13}\text{CCH}/\text{C}^{13}\text{CH-H}_2$ rate coefficients

Resolution of the Time-independent Schrödinger equation through
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- *ab initio* calculations
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Resolution of the Close-Coupling equations
→ describe the nuclear interaction between colliders

- cross sections $\sigma(E_{kin})$
- rate coefficients ($\sim \int_0^\infty \sigma(E_{kin})dE_{kin}$)

Most accurate approach ✓

Most expensive one ✗

Number of channels: N

→ Mem $\propto N^2$, time $\propto N^3$

Potential energy surface

- Linear rigid rotor approximation
- 4D PES¹
- RCCSD(T)/aVQZ method
- Calculations are done with the MOLPRO code²
- The PES was expanded in bispherical harmonics

→ PES will be used for isotopologues

¹Dagdigan, J. Chem. Phys. 148, 024304 (2018)

²Werner, Molpro, a package of ab initio programs, version 2015.1, 2015

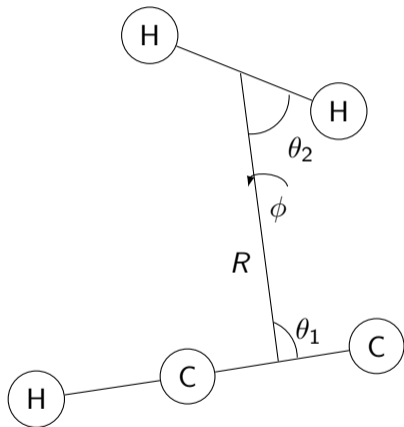


Figure: C₂H-H₂ representation in Jacobi coordinates

Hyperfine structure of ^{13}C isotopologues

Open-shell molecules with a $^2\Sigma^+$ ground electronic state

- non zero total electronic spin $S = \frac{1}{2}$

$$\Rightarrow \hat{J} = \hat{N} + \hat{S}$$

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- non zero nuclear spin from ^{13}C atom $I_1 = \frac{1}{2}$

$$\Rightarrow \hat{F}_1 = \hat{J} + \hat{I}_1$$

- non zero nuclear spin from hydrogen atom $I_2 = \frac{1}{2}$

$$\Rightarrow \hat{F} = \hat{F}_1 + \hat{I}_2$$

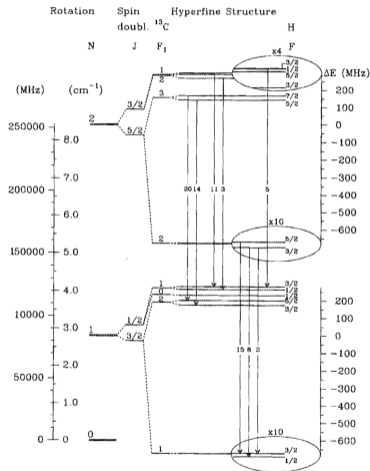
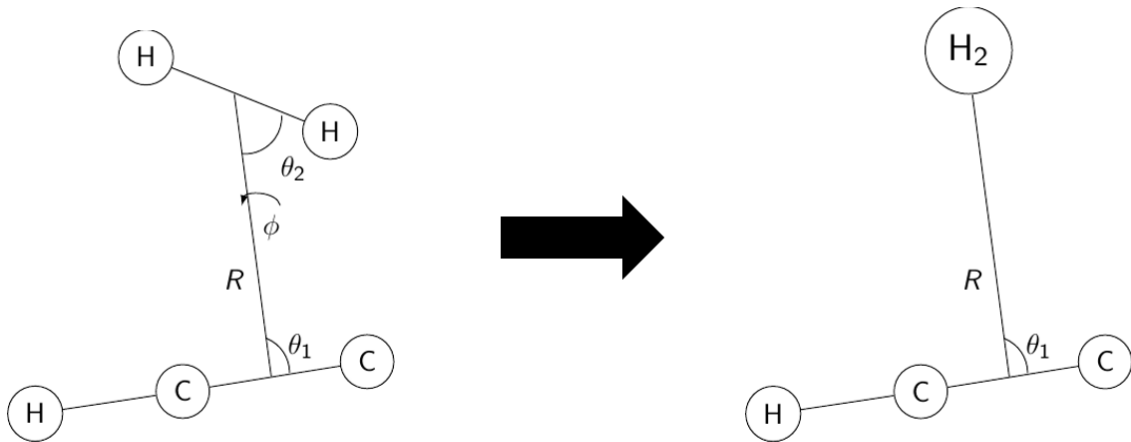


Figure: Example of hyperfine structure of ^{13}CCH 15 / 21

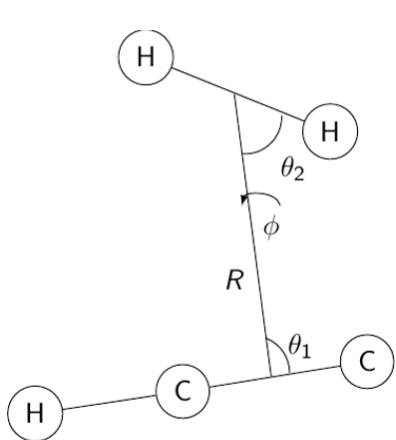
Reduced dimensionality approximation



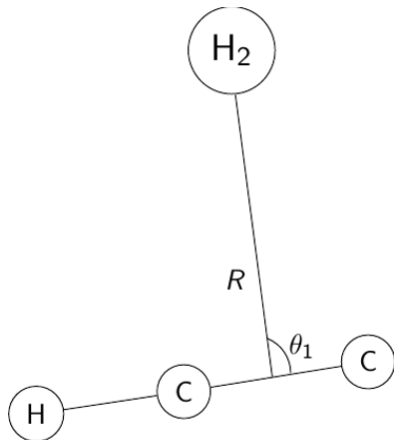
Number of basis functions: 174

Mem \sim 70Gb

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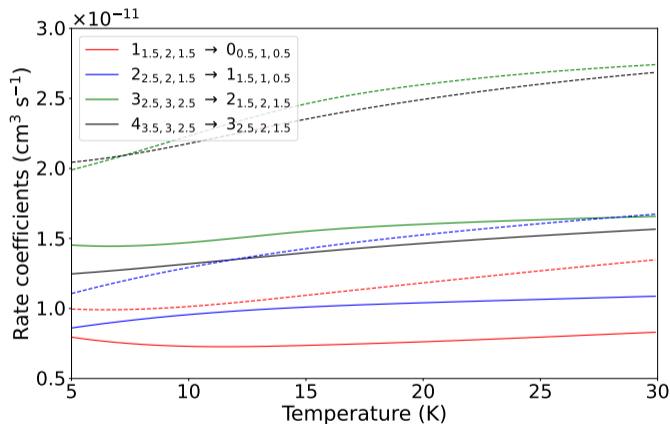


Number of basis functions: 174
Mem \sim 70Gb



Number of basis functions: 13
Mem \sim 6Gb

Preliminary results for isotopologues



- 4D \rightarrow 2D PES
- Resolution of the close-coupling equations
- Calculations have been done using HIBRIDON scattering code¹
- Extraction of the cross sections \rightarrow determination of the rate coefficients

¹Alexander 2023, submitted

Figure: Temperature dependance of rate coefficients of ¹³CCH and C¹³CH with H₂ for $N_{j,F_1,F} \rightarrow N'_{j',F'_1,F'}$ transitions

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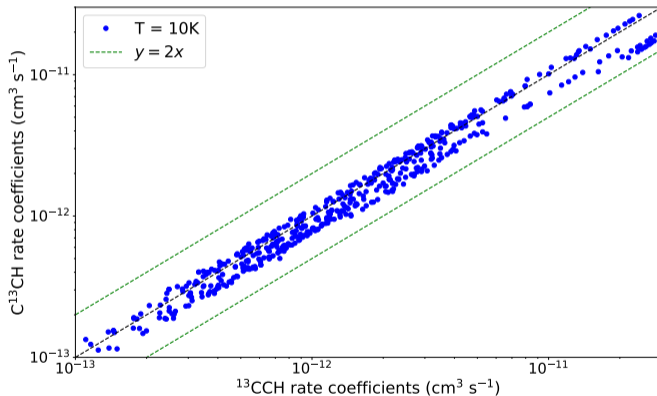


Figure: Systematic comparison at 10K of C^{13}CH rate coefficients with ^{13}CCH ones

Conclusion and perspectives

- First preliminary $^{13}\text{CCH-}$ and $\text{C}^{13}\text{CH-H}_2$ rate coefficients
- Moderate isotopic effect for isotopologues rate coefficients (deviations $\sim 20\text{-}30\%$)
- Extend the range of temperatures where these molecules are detected
- These data are expected to be used in radiative transfer modeling

Acknowledgments

