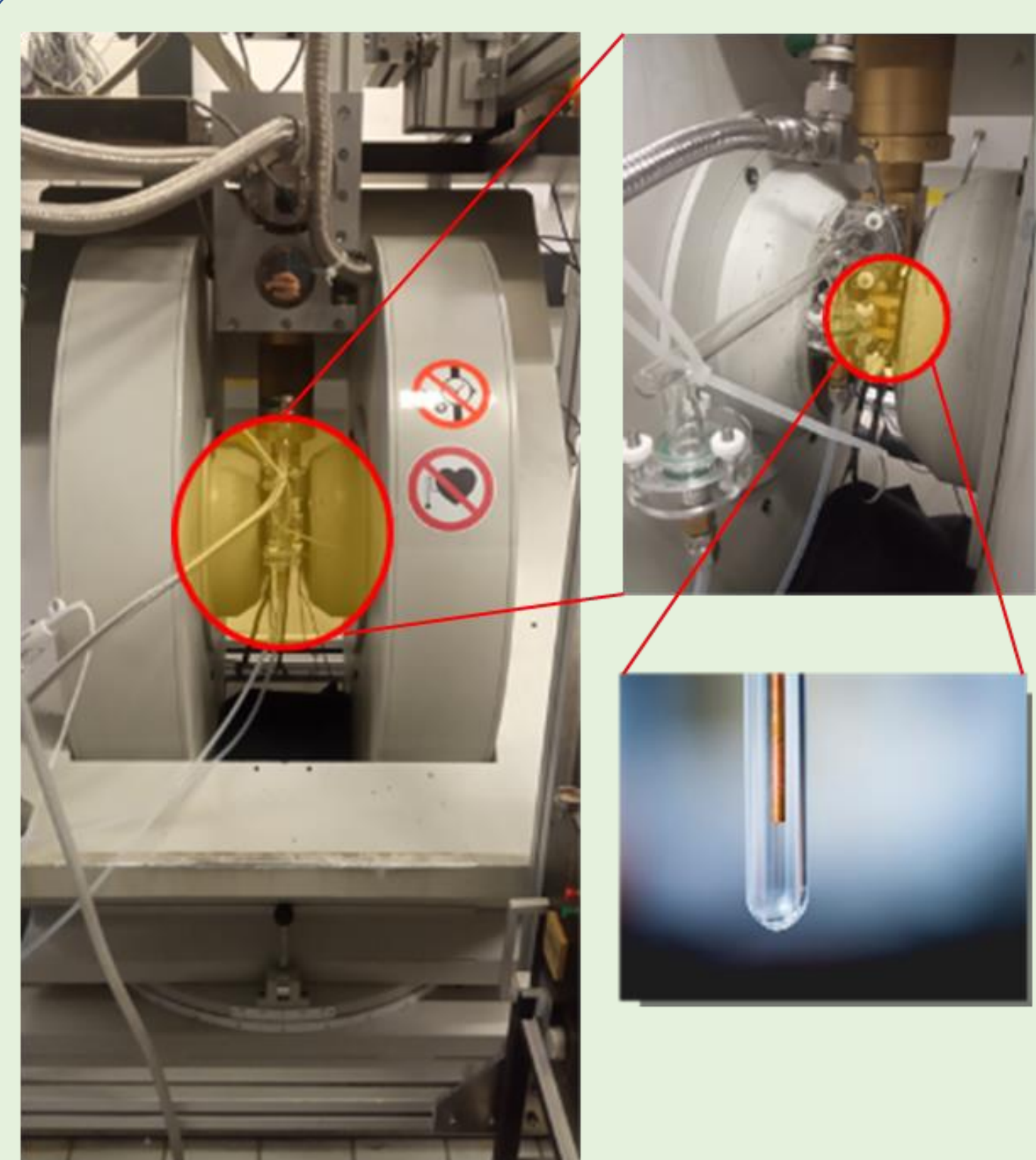


Radical and iCOM Formation From VUV Photolysis of H₂O:CO Interstellar Ice Analogues: an EPR Coupled to IR and QMS-TPD Study

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Bochum EPR experiment

Introduction

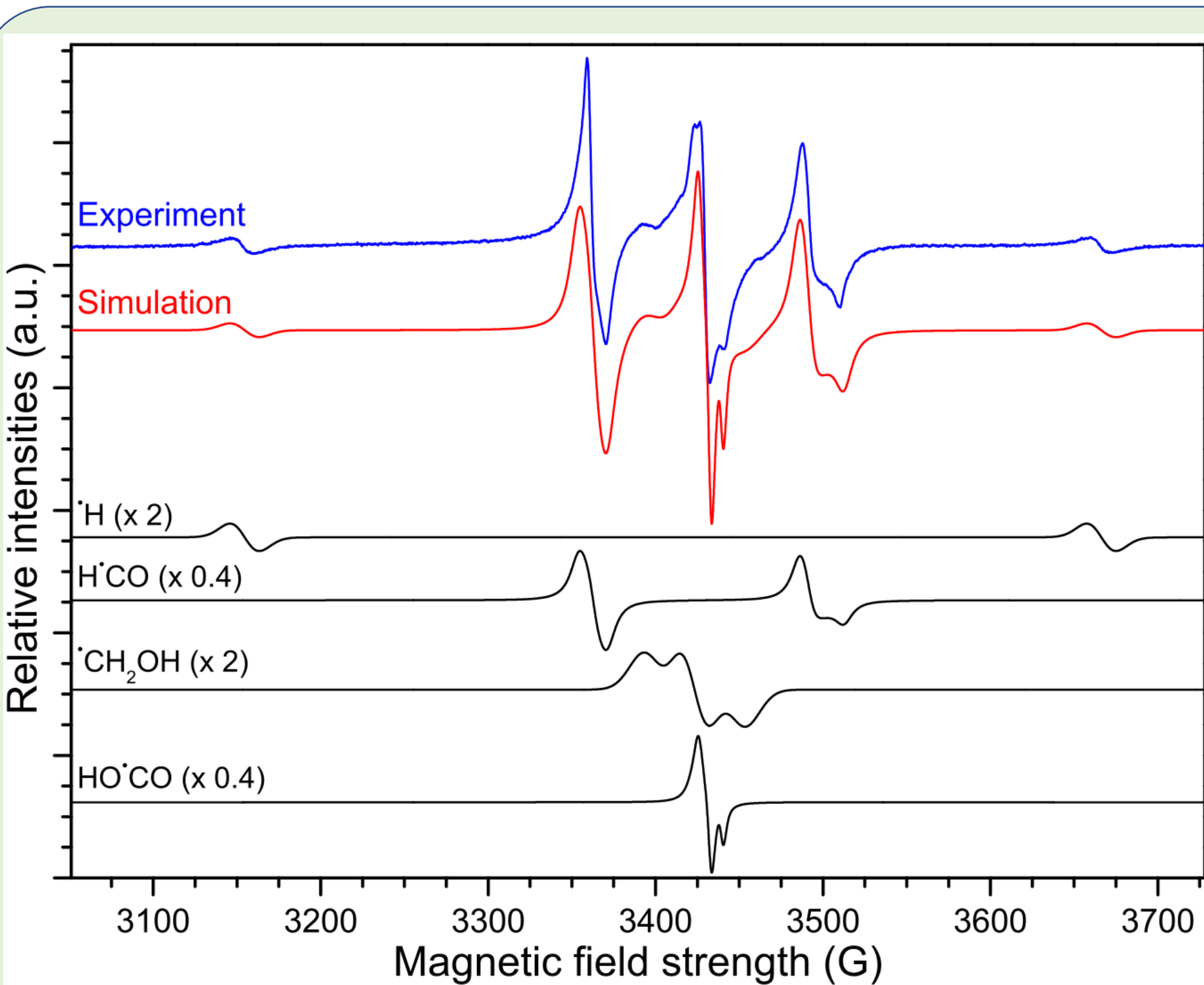
- COM formation mechanisms are not well established and could take place either in gas or solid phase. [1,2]
- We developed an unique experimental procedure allowing the detection of intermediary (radical) species and stable products in the same experimental conditions. [3]
- This work aims to apply this methodology to interstellar ice analogues with the astro relevant CO/H₂O system.
- We propose **solid phase formation mechanisms** of some carboxylic acids under VUV photolysis at Lyman- α wavelength.



RING experiment

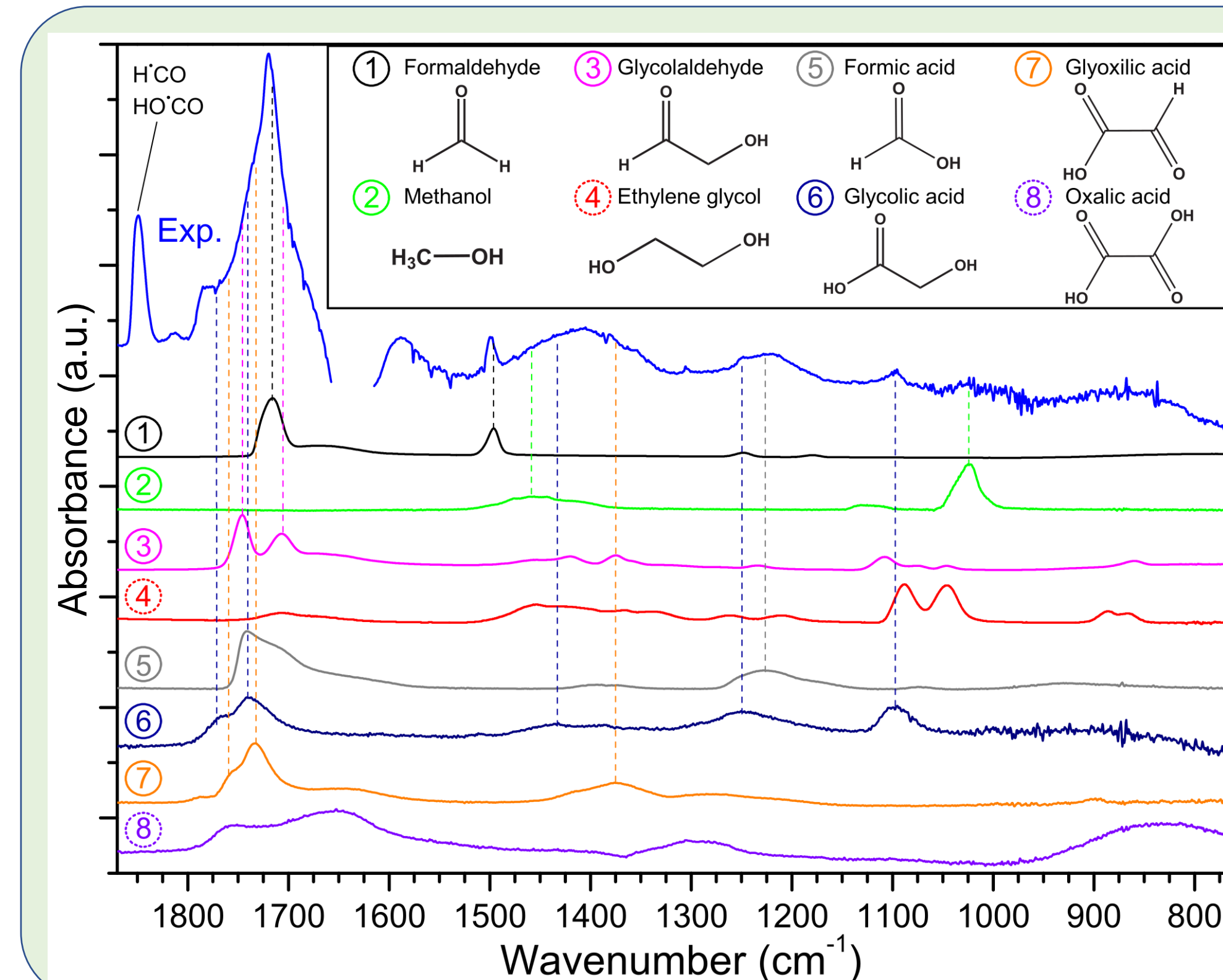
Experimental procedure

- CO/H₂O = 1/1 deposition at 4 K (Bochum) or 12 K (RING).
- Photolysis (121.6 nm) and EPR/IR acquisition at 4 K/12 K.
- QMS-TPD acquisition (EI, 70 eV) between 160 and 300 K.



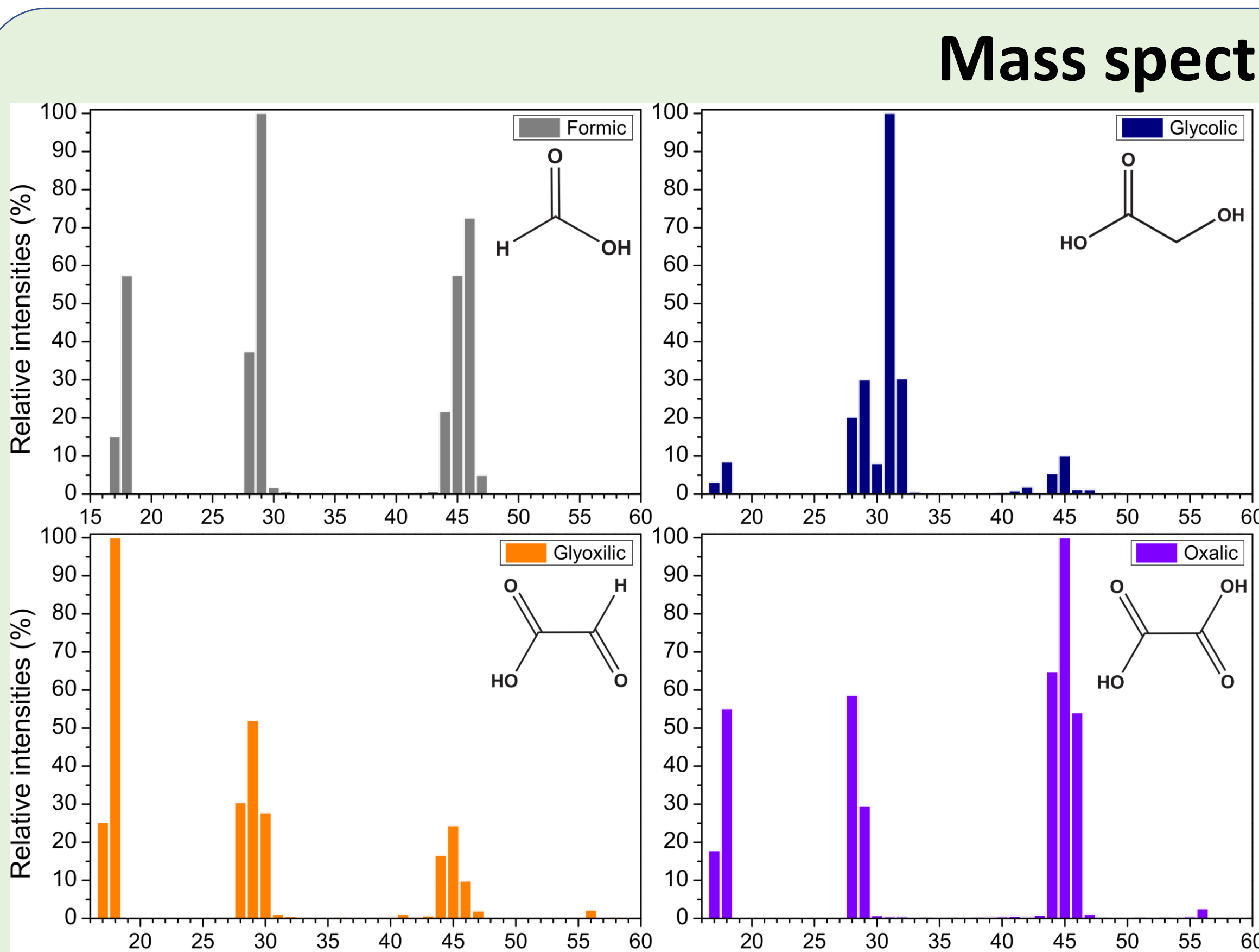
EPR detection of radical intermediates

- Radicals simulated with EasySpin in MATLAB.
- Detected radicals: **H[•], H[•]CO, [•]CH₂OH, HO[•]CO.**
- Intensities proportionnal to species quantity.
- Two major intermediaries: HO[•]CO & H[•]CO.



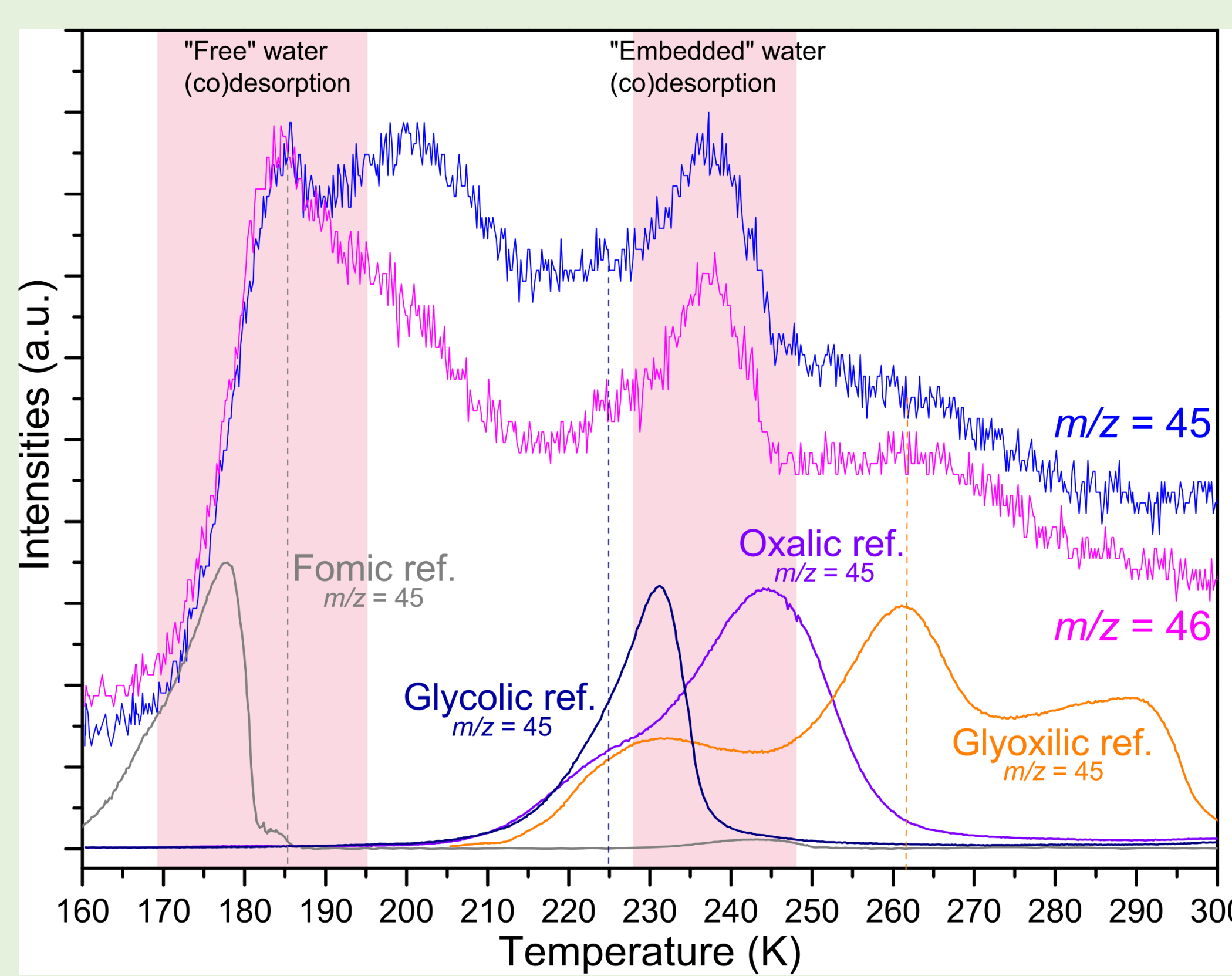
IR detection of radicals and COMs

- Two detectable radicals: HO[•]CO & H[•]CO.
- CO hydrogenation products [4]:
CO $\xrightarrow{2H}$ H₂CO $\xrightarrow{2H}$ CH₃OH
- Strong hints: Formic and glycolic acids.
- Not conclusive: GA, EG, oxalic and glyoxilic acids.

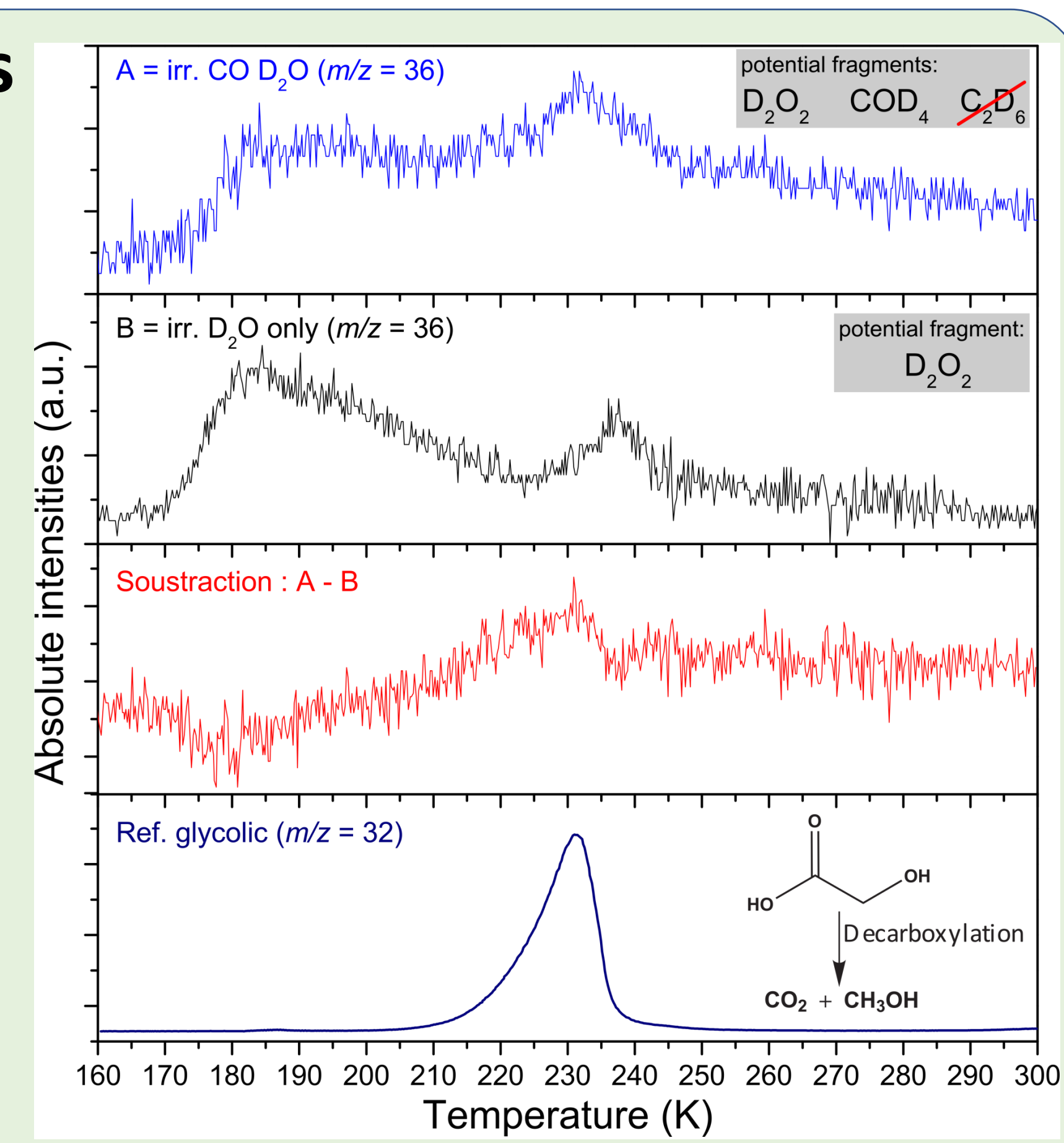


Mass spectrometry (QMS-TPD) detection of products

- RING apparatus references.
- All acids share same m/z fragments.
- m/z=46 > m/z=45 only for FA.
- m/z=31 & m/z=32 only for glycolic acid.



- Codesorption of all acids between 160 and 300 K.
- [170K ; 190K]: m/z=45 = m/z=46 → Mainly FA desorbing.
- Some concordances for glycolic and glyoxilic acids.



- Glycolic m/z=32 (COH₄) → m/z=36 (COD₄).
- [210K ; 240K]: desorption of a COD₄ fragment correlated to glycolic reference.

	H [•]	H [•] CO	[•] CH ₂ OH	HO [•] CO
H [•]	H ₂	<chem>H-C(=O)-H</chem>	<chem>HO-CH2-OH</chem>	<chem>HO-C(=O)-H</chem>
H [•] CO		<chem>H-C(=O)-H</chem>	<chem>H-C(=O)-CH2-OH</chem>	<chem>HO-C(=O)-H</chem>
[•] CH ₂ OH			<chem>HO-CH2-CH2-OH</chem>	<chem>HO-C(=O)-CH2-OH</chem>
HO [•] CO				<chem>HO-C(=O)-H</chem>

 Detected molecules
 Not enough evidence
 No possible conclusion

Conclusion

- ✓ Detection of at least four radical intermediary species from CO/H₂O VUV photolysis: **H[•], H[•]CO, [•]CH₂OH, and HO[•]CO.**
- ✓ Two carboxylic acids can be formed in solid state by radical recombination:
H[•] + HO[•]CO → HCOOH (FA) & [•]CH₂OH + HO[•]CO → HOCH₂COOH (glycolic acid).
- ✓ Glyoxilic & oxalic acids could also be formed but more experiments are needed.
- ✓ Formic acid has been detected in the ISM [5] and interstellar ices [6]. Glycolic acid has not (yet) been observed, let's search for this molecule 😊.

References

[1] K.-J. Chuang et al., *MNRAS*. **2017**, 467, 2552. [2] D. Skouteris et al., *ApJ*. **2018**, 854, 135. [3] A. Gutiérrez-Quintanilla et al., *MNRAS*. **2021**. [4] T. Hama and N. Watanabe, *Chem. Rev.* **2013**, 113, 8783. [5] B. Zuckerman et al., *ApJ*. **1971**, 163, L41. [6] A. C. A. Boogert et al., *ApJ*. **2008**, 678 (2), 985.

