Nuclear-spin astrochemistry: from laboratory to observations (and *vice versa*)

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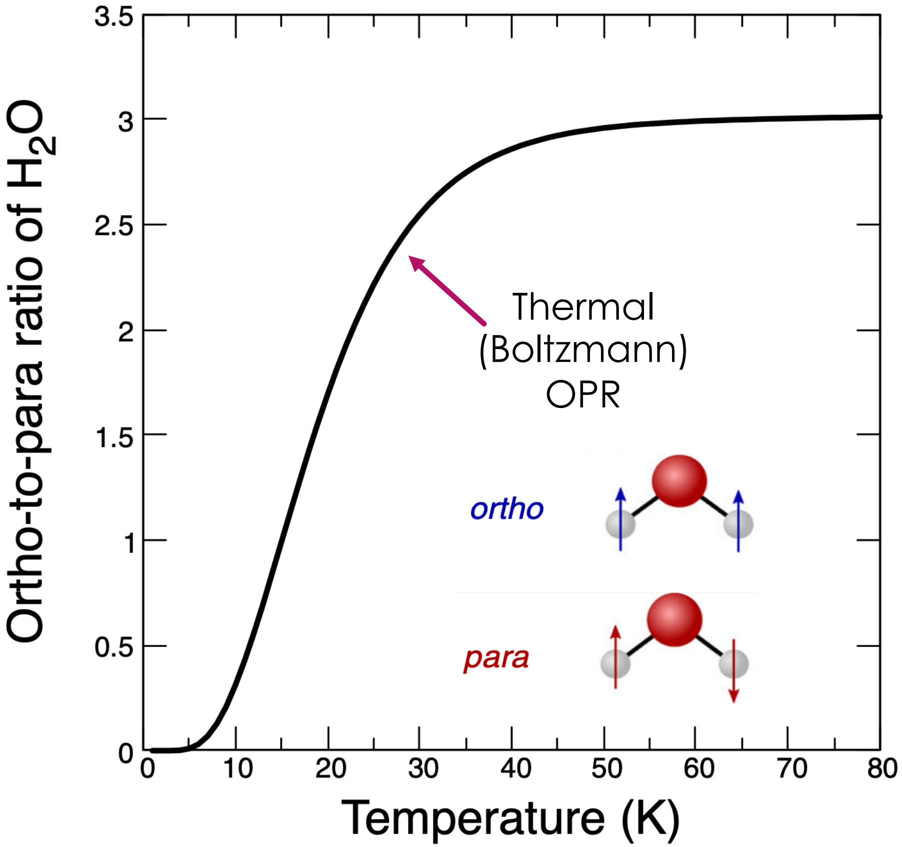
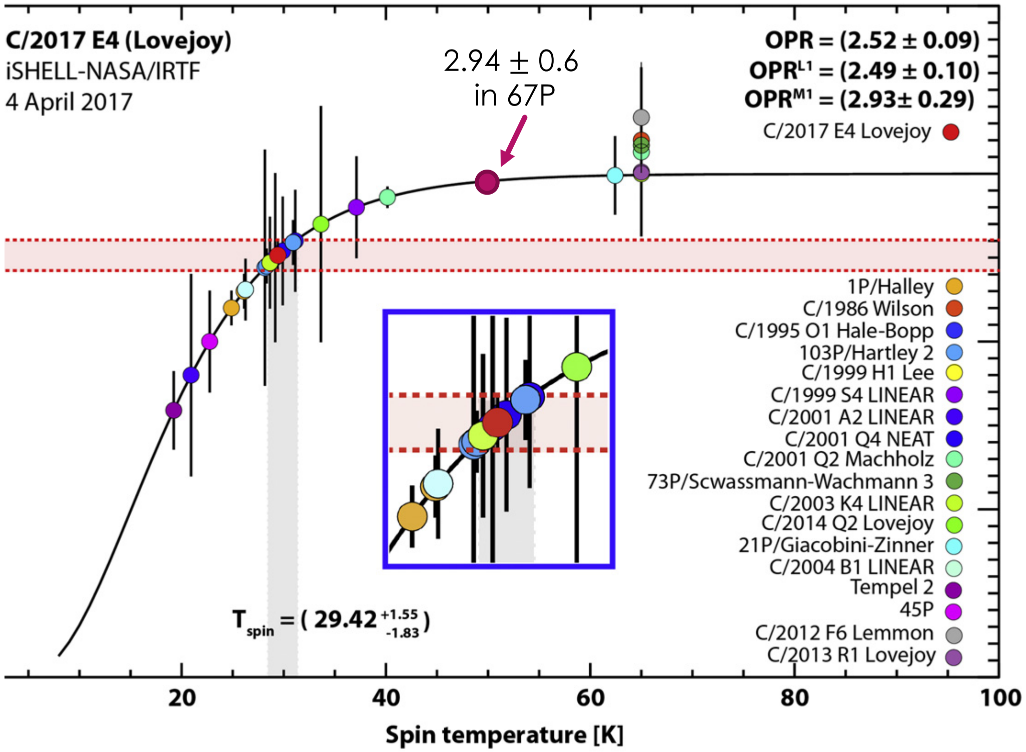
COLLOQUE PCMI – BORDEAUX – 30 OCTOBER 2024

The ortho-to-para ratio (OPR) of H_2O



- At room temperature, H_2O consists of ¾ ortho-H_2O (I=1) and ¼ para-H_2O (I=
- Gas-phase conversion by radiation or inelastic collisions is extremely slow
- The OPR of H_2O at formation should be preserved in the gas phase

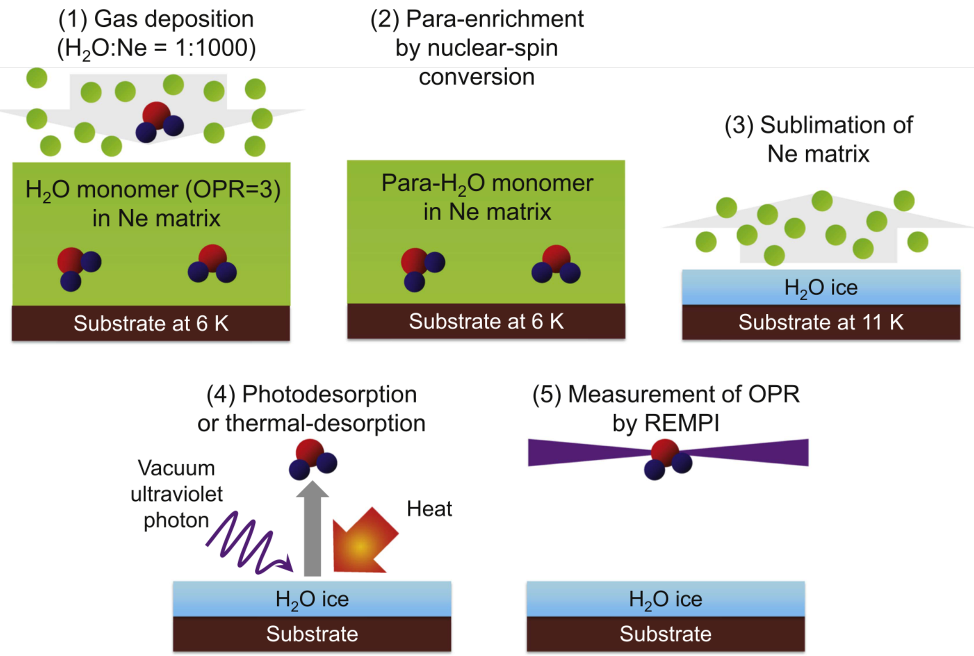
The OPR of H_2O in comets



Faggi et al. (2018) + Cheng et al. (2022)

- The 'spin' temperatures of H_2O in com are ~ 30 K on average
- A probe of the formation history of cometary ices ? (Mumma et al. 1986)
- But no laboratory evidence until recer

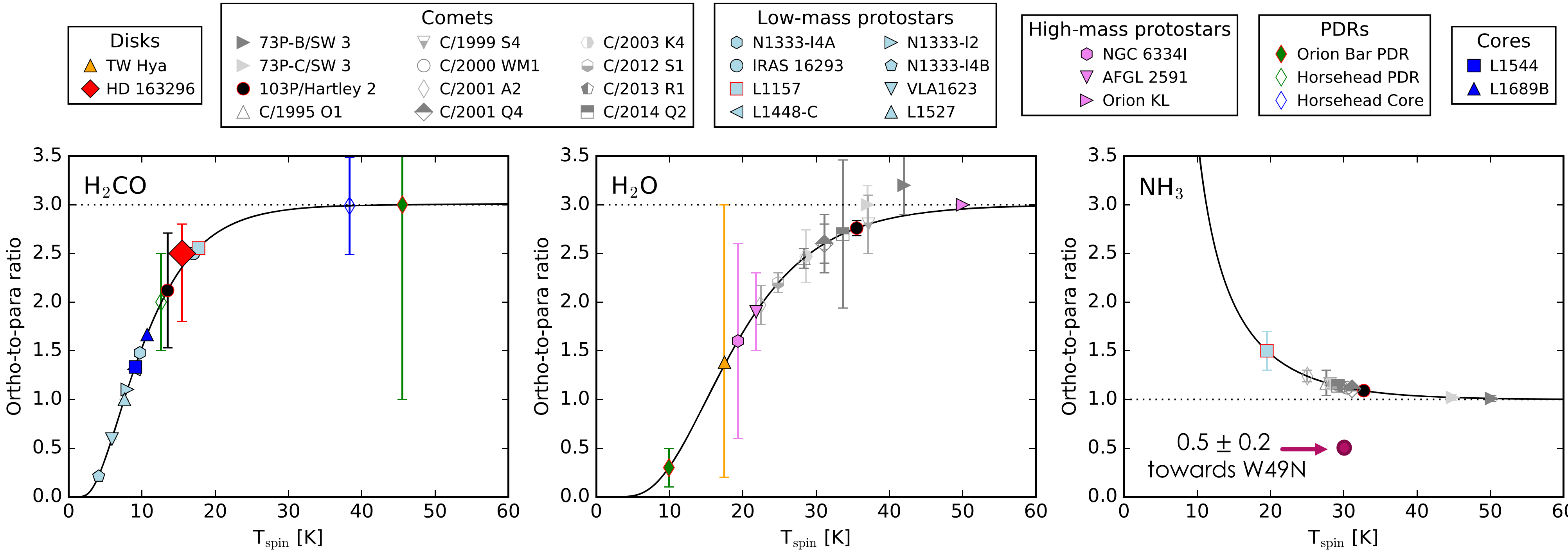
The OPR of H_2O in laboratory ices



Hama et al. (2018)

- H_2O molecules photo or thermally des
from ice have a statistical OPR of 3
- A low OPR does not reflect the format
temperature
- Underlying interconversion mechanims
(Turgeon et al. 2017)

The OPR of H_2CO, H_2O and NH_3: from clouds to disks



Guzman et al. (2018) + Persson et al. (2012)

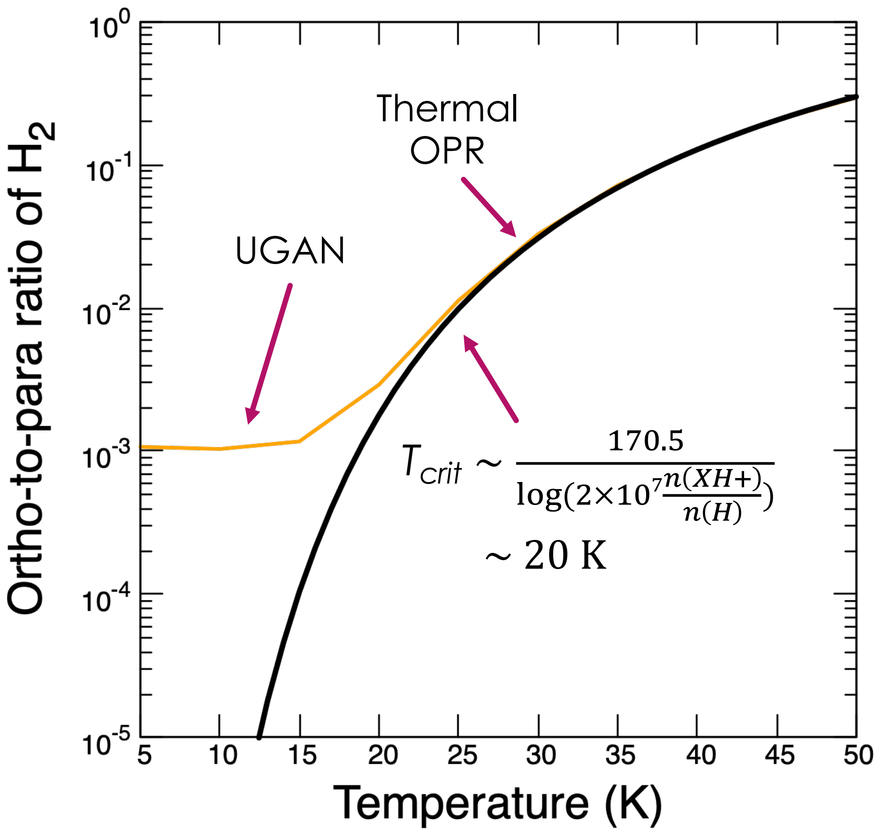
Alternative to the formation on dust: gas-phase reactions !

drogen abstraction reactions
ample)

- $OH^+ + p\text{-}H_2 \longrightarrow (H_3O^+)^* \longrightarrow p\text{-}H_2O^+ + H$ 1/2
- $OH^+ + p\text{-}H_2 \longrightarrow (H_3O^+)^* \longrightarrow o\text{-}H_2O^+ + H$ 1/2
- $OH^+ + o\text{-}H_2 \longrightarrow (H_3O^+)^* \longrightarrow p\text{-}H_2O^+ + H$ 1/6
- $OH^+ + o\text{-}H_2 \longrightarrow (H_3O^+)^* \longrightarrow o\text{-}H_2O^+ + H$ 5/6

- The conservation of the total nuclear s imposes selection rules (Quack 1977)
- Full scrambling of nuclei is assumed
- Experimental support: state-to-state control of 2 KRb → K_2 + Rb_2 (Hu et al. 2

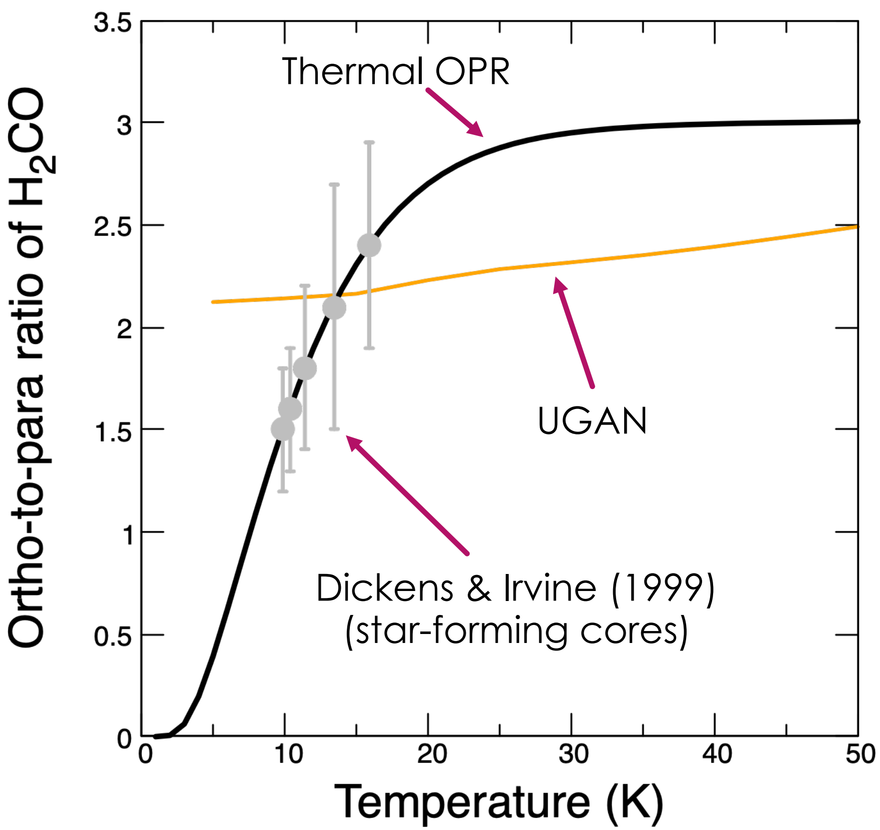
The UGAN network for the cold ISM



Faure et al. (2013)

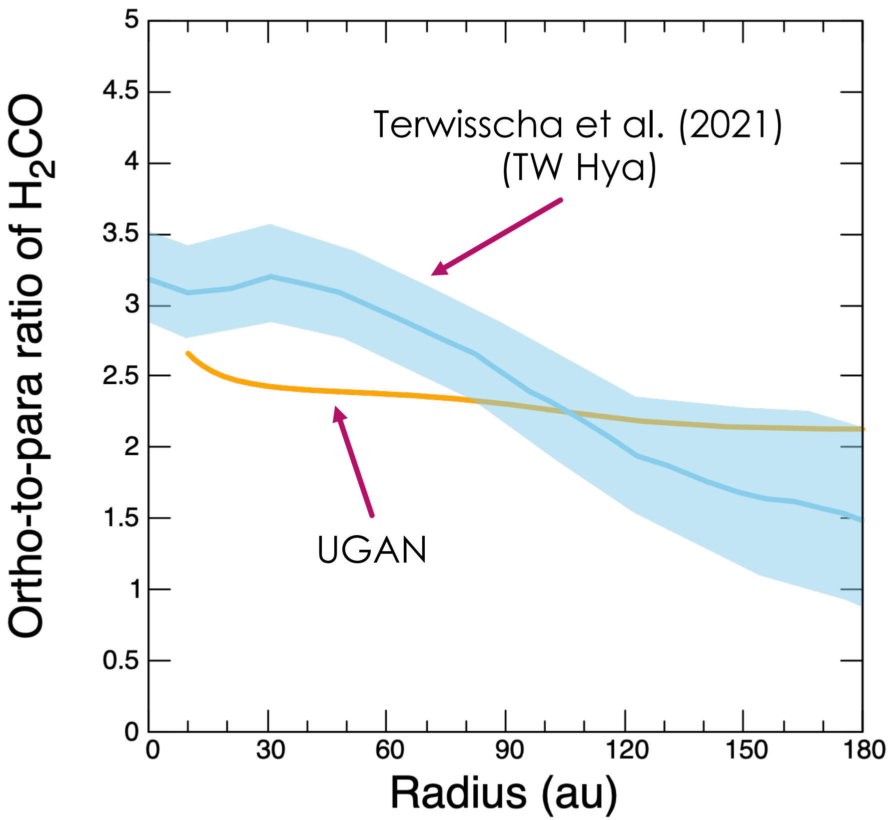
- The UGAN network (Hily-Blant et al. 20
  - 219 species / 3427 reactions (gas + ice
  - Spin isomers of hydrides and H_2CO
- We predict a para-rich H_2 gas, in agreement with indirect evidences
- Deviation from a thermal OPR is due t barrier of 170 K in p-H_2 + XH^+ ⇆ o-H_2 +

The OPR of H_2CO in the cold ISM



- Gas-phase formation via the reaction $CH_3 + O \longrightarrow H_2CO + H$ (k =6.9×10^{-11} cm^3
- We predict an OPR of H_2CO ~ 2.3, in li with values in star-forming cores
- The OPR of H_2CO (and H_2O, NH_3, etc.) driven by the low OPR of H_2

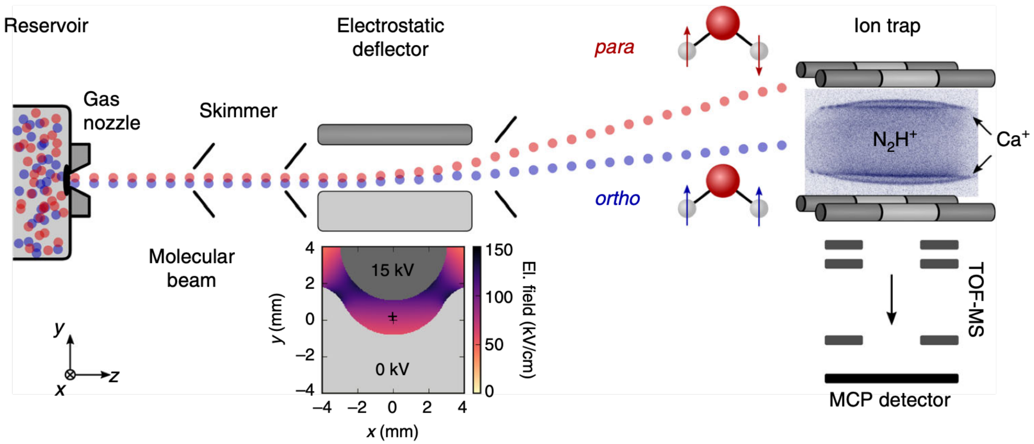
The OPR of H_2CO in TW Hya



Gaillard et al. in preparation

- Thanks to ALMA the emission of H_2CO be spatially resolved in protoplanetary
- In TW Hya, the OPR of H_2CO varies between 3 ($R < 60$ au) and 1.5 ± 0.6
- Our model reproduces the OPR at R>8 suggesting a gas-phase formation of H

Conclusions and perspectives



Kilaj et al. NatCom (2018); Toscano CHIMIA (2024)

- Conclusions:
  - OPRs do not probe 'formation' temper
  - Anomalous (non-statistical) OPRs can b explained by gas phase chemistry
- Perspectives:
  - Thermalization gas phase processes m important (e.g. NH_2 + H, Le Gal et al. 20
  - The different reactivity of spin isomers w ions can now be explored experiment

Acknowledgements

- **IPAG**: A. Bacmann, M. Gaillard, P. Hily-Blant, R. Le Gal, C. Rist, M. Tanious
- **MONARIS**: X. Michaut, J.H. Fillion
- **Basel**: J. Toscano
- **Bordeaux**: T. Stoecklin