Hydrides, including water and H₂

David Neufeld Johns Hopkins University

Hydrides (for the purpose of this talk): molecules containing one or more hydrogen atoms and one or fewer heavier atoms

Importance of hydrides

(see 2016 ARAA article by Gerin et al.)

Hydrides lie at the root of interstellar chemistry, and are key intermediaries in the pathways to more complex molecules

Small moment of inertia → large rotational constant → rotational transitions primarily in the far-IR/submm regime (mid-IR for H₂) → need *Herschel* and SOFIA

H₂ is the most abundant molecule in the Universe and is a key molecular coolant of gas above ~ 100 K

H₂O is considered THE key ingredient for life

Because their formation and destruction is governed by a *relatively small* network of chemical processes, hydrides are very valuable probes of the environment in which they are found

Hydrides as diagnostic probes

In the interstellar medium

- 1) CH, HF → total H₂ column density
- 2) CH⁺, SH, SH⁺, H₂O, OH \rightarrow warm gas in shocks and TDRs
- 3) OH⁺, H₂O⁺, ArH⁺, H₃⁺ \rightarrow ionization by cosmic rays
- 4) ArH⁺, OH⁺/H₂O⁺, HCl⁺/H₂Cl⁺ ratios → local H₂ fraction
- 5) Ortho/para ratios → clock for measuring ages

In protoplanetary disks

HD → total gas mass (e.g. Bergin et al. 2013, Mihkel Kama's talk) H₂O (line profiles for kinematic tomography) → the "snow line"

In comets

HDO, $H_2O \rightarrow$ delivery of volatiles to inner rocky planets

Previous contributions of SOFIA

With GREAT

- First detections of astrophysical SH (Neufeld+ 2012, 2015), OD (Parise+ 2012), HeH+ (Gusten+ 2019), para-H₂D+ (Brunken+ 2014)
- First detection of H₂O water masers (Neufeld+ 2017, Herpin+ 2017)

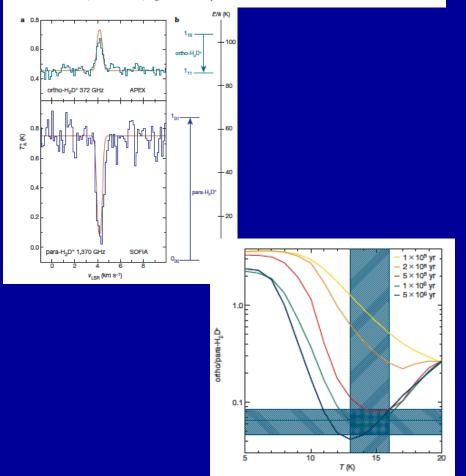
GREAT discoveries of para-H₂D⁺ and HeH⁺

LETTER

doi:101028/nature12024

H₂D⁺ observations give an age of at least one million years for a cloud core forming Sun-like stars

Sandra Brünken¹, Olli Sipilä^{2,3}, Edward T. Chambers¹, Jorma Harju², Paola Caselli^{3,4}, Oskar Asvany¹, Cornelia E. Honingh¹, Tomasz Kamiński², Karl M. Menten⁵, Jürgen Stutzki¹ & Stephan Schlemmer¹

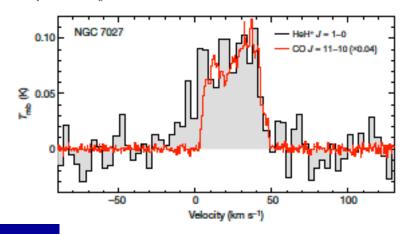


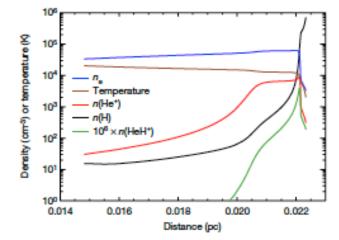
LETTER

https://doi.org/10.1038/s41586-019-1090-x

Astrophysical detection of the helium hydride ion HeH⁺

Rolf Güsten^{1*}, Helmut Wiesemeyer¹, David Neufeld², Karl M. Menten¹, Urs U. Graf⁴, Karl Jacobs³, Bernd Klein^{1,4}, Oliver Ricken¹, Christophe Risacher^{1,5} & Jürgen Stutzki³





Previous contributions of SOFIA

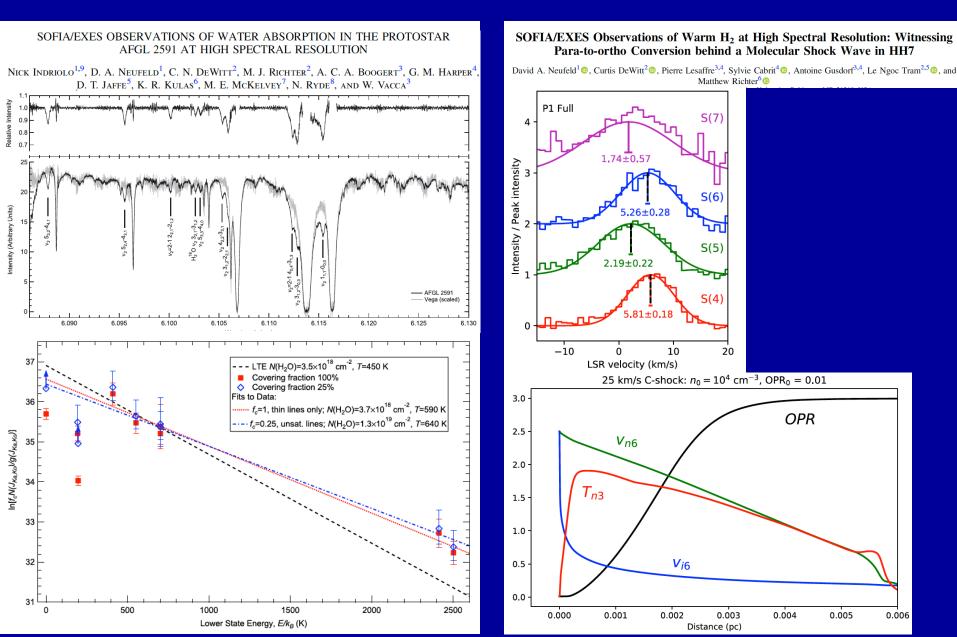
With GREAT

- First detections of astrophysical SH (Neufeld+ 2012, 2015), OD
 (Parise+ 2012), HeH+ (Gusten+ 2019), para-H₂D+ (Brunken+ 2014)
- First detection of THz water masers (Neufeld+ 2017)

With EXES

- Detection of H₂O vibrational absorption toward massive protostars (Indriolo+ 2015, 2020) → missing oxygen problem
- First velocity-resolved observations of H₂ pure rotational emissions from shocks → compelling direct evidence for continuous-type 'C'-type shocks (Neufeld+ 2019)

EXES observations of H₂O and H₂



Future prospects with current instrumentation

SOFIA PROPOSAL 08_0038

HyGAL: characterizing the Galactic interstellar medium with hydrides

Investigator	Institution	Investigator	Institution
Prof. David Neufeld	Johns Hopkins University	Dr. Volker Ossenkopf-Okada	University of Cologne
Prof. Peter Schilke	University of Cologne	Dr. Patrick Hennebelle	CEA
Prof. Amiel Sternberg	Tel Aviv University	Dr. Alvaro Sanchez-Monge	University of Cologne
Dr. Benjamin Godard	LERMA	Dr. Shmuel Bialy	Harvard-Smithsonian Center for Astrophysics
Dr. Darek Lis	Caltech	Dr. Daniel Seifried	University of Cologne
Dr. Davide Elia	INAF	Dr. Paule Sonnentrucker	STScI
Prof. Edith Falgarone	ENS	Dr. Valeska Valdivia	CEA
Prof. Maryvonne Gerin	ENS	Prof. Stefanie Walch	
Dr. Sergio Molinari	INAF		University of Cologne
Dr. Mark Wolfire	University of Maryland	Dr. Friedrich Wyrowski	MPIfR
Dr. Nick Indriolo	STScI	Prof. Karl Menten	MPIfR
DI. NICK HIGHOIO	51501	Dr. Ronan Higgins	University of Cologne
		Dr. Helmut Wiesemeyer	MPIfR

HyGAL

Cycle 8/9 SOFIA Joint Legacy Program with GREAT

4 GREAT: simultaneous observations of H₂O⁺, ArH⁺, OH⁺, SH, OH

LFA: observations of CH (2 THz lines) and C+

HFA: observations of O

Absorption line spectroscopy towards 25 continuum sources (from the Hi-GAL source list)

Time allocated: 82 hours

HyGAL

Questions to be addressed

- How does the density of low-energy cosmic-rays vary within the Galaxy. To what extent does the cosmic ray density vary statistically on small scales and systematically with Galactocentric distance and gas column density?
- What is the distribution function of H₂ fraction in the ISM in different environments?
- What is the nature of interstellar turbulence, and what mechanisms lead to its dissipation?

Future instrumentation

All these results have been obtained from observations with high spectral resolution $(\lambda/\Delta\lambda \sim 80,000 \text{ or above}).$

Current high-resolution instruments, and their spectral coverage relevant to hydrides

GREAT: 116 – 610 μm: transitions connecting to the ground state (mainly absorption)

EXES: $5 - 28 \mu m$: H₂ rotational emissions, H₂O vibrational

Future instrumentation

Gap in high-resolution coverage: 28 – 116 μm

A general purpose instrument (i.e. fully-tunable) covering these two octaves at high spectral resolution would provide access to emission from excited states of hydrides in gas above ~ 100 K Bolometric detectors could provide improved sensitivity on either side of this gap

Key species: H₂O, OH, HD, CH⁺

Key environments: protoplanetary disks, solar system planets and comets (talks by Stacey, Kama, Lis) but also interstellar shocks and evolved stars

This spectral region also contains key atomic transitions, expecially the [SiII] $35~\mu m$ line (analog of the [CII] $158~\mu m$ line)

ISO/SWS spectrum of VY CMa

 $\lambda/\Delta\lambda = 2000$

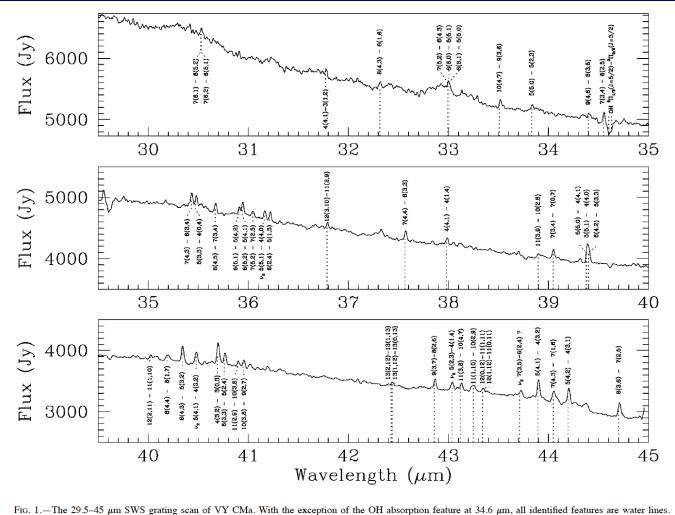
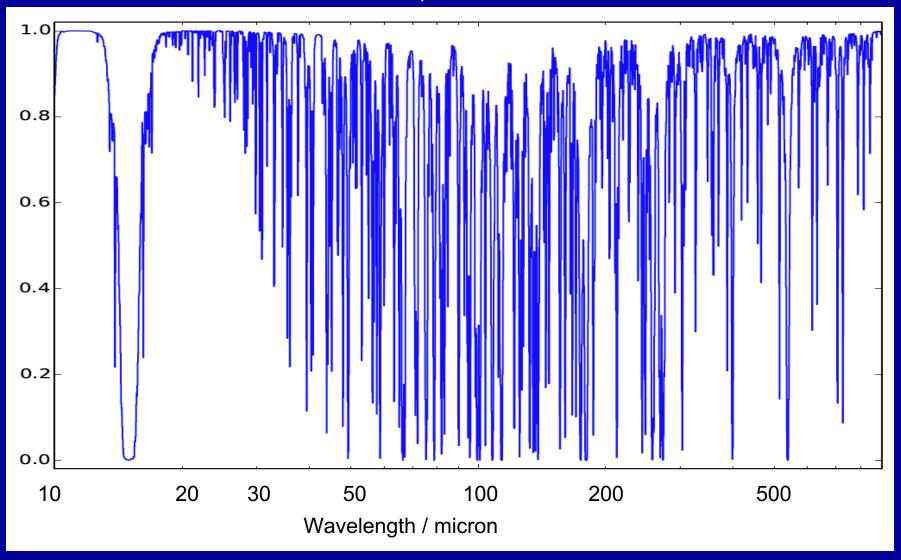
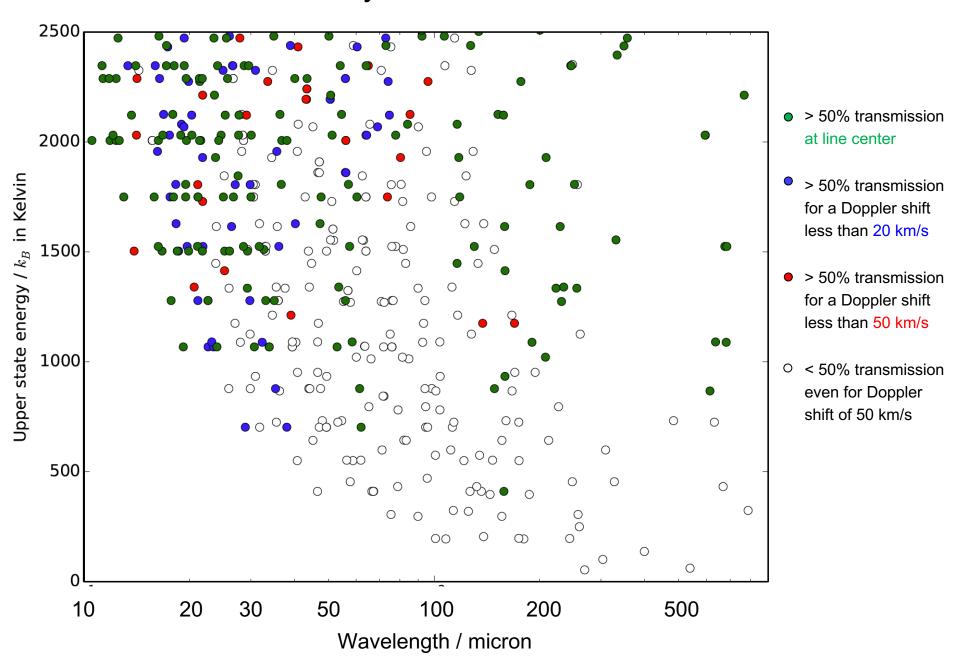


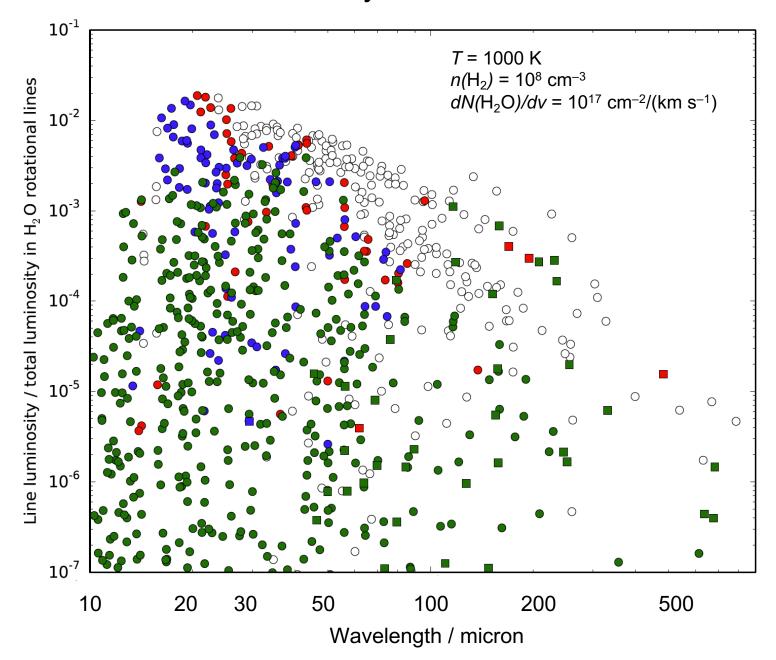
Fig. 1.—The 29.5-45 μm SWS grating scan of VY CMa. With the exception of the OH absorption feature at 34.6 μm, all identified features are water lines.

Water lines at airplane altitude

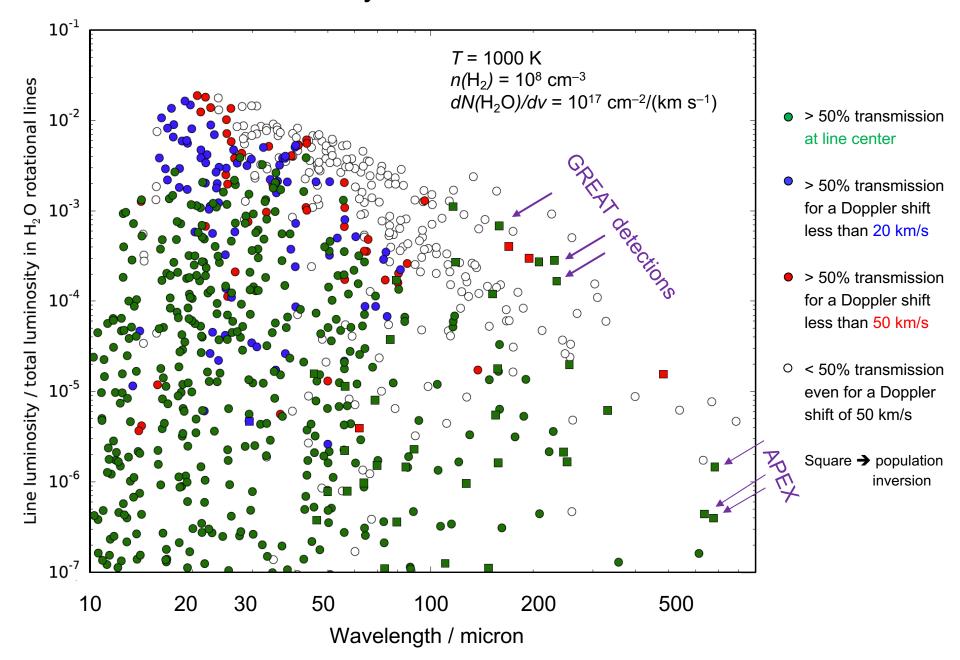
Atmospheric transmission at 41,000 ft (elevation= 45 deg, PWV = 7μ m, ATRAN code, smoothed to R=500)

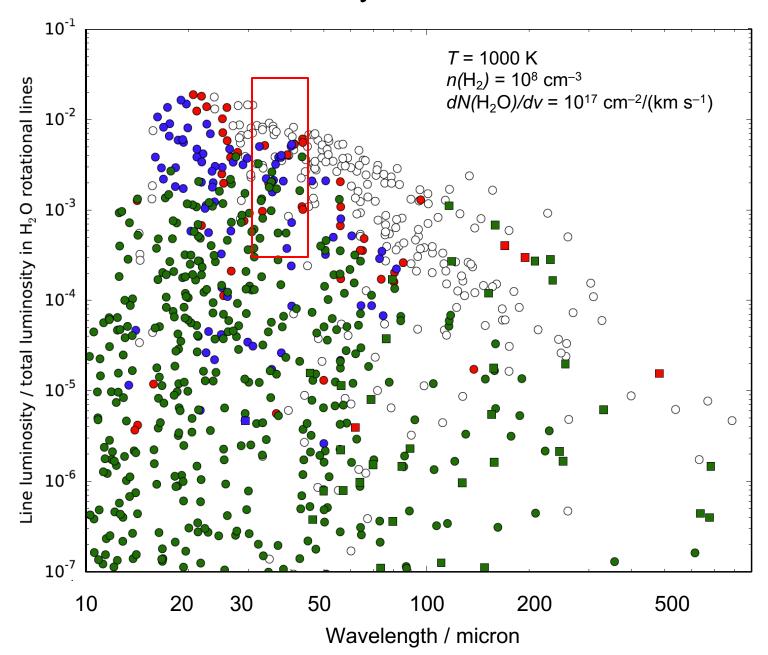






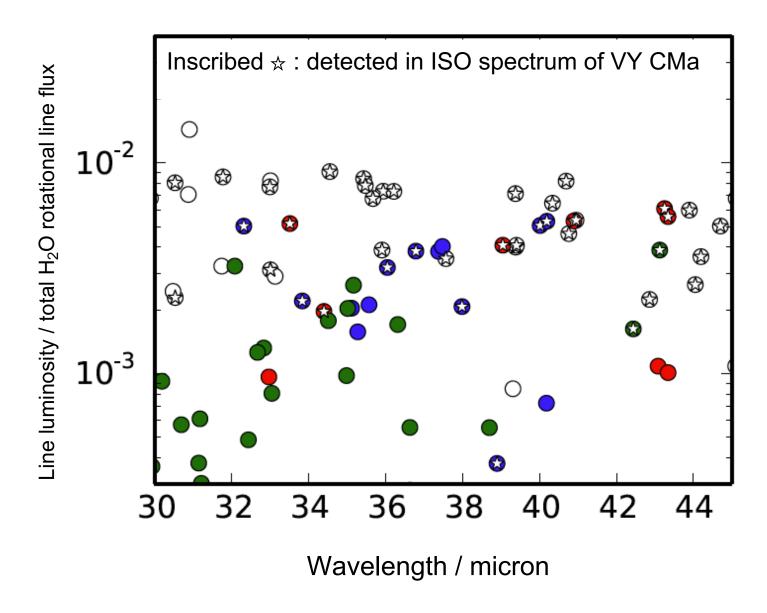
- > 50% transmission at line center
- > 50% transmission for a Doppler shift less than 20 km/s
- > 50% transmission for a Doppler shift less than 50 km/s
- < 50% transmission even for a Doppler shift of 50 km/s
 - Square → population inversion



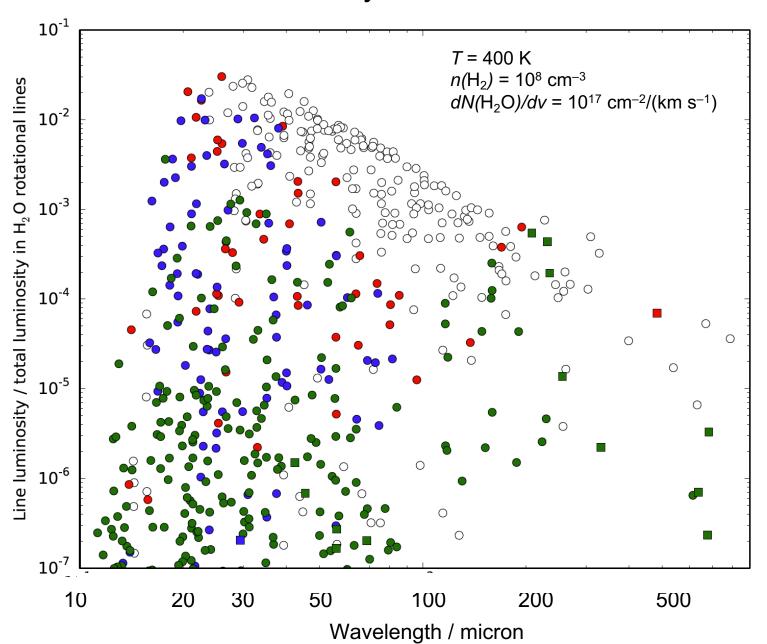


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Summary

Hydrides are key probes of astrophysical sources and processes: previous high-spectral resolution spectroscopy with EXES and GREAT has produced high impact science

Much still remains to be done with existing instrumentation (e.g. HyGAL, survey of H₂ emission from shocks...)

A general-purpose high-resolution spectrometer bridging the gap between EXES and GREAT – and improving the sensitivity with incoherent detectors (bolometers) – would make SOFIA a unique facility for probing emission from hydrides in protoplanetary disks, shocks, evolved stars....