SOFIA/EXES observations of warm H_2 at high spectral resolution:

witnessing para-to-ortho conversion behind a molecular shock wave in HH7

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Paper: Neufeld et al. 2019, ApJ Letters (arXiv: 1095.10381)


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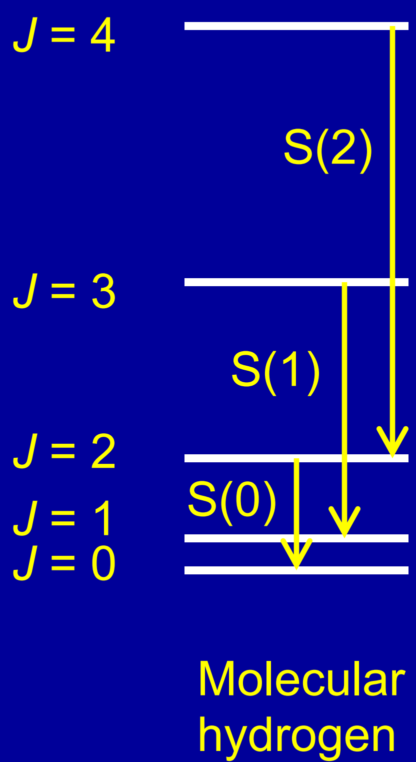
H_2 rotational structure

Absence of dipole moment ➔ $\Delta J = -2$ selection rule



H_2 rotational structure

The hydrogen nuclei are two identical spin-1/2 fermions
➔ wavefunction must be antisymmetric with respect to interchange of those nuclei

For the total spin = 1 state (ortho-H_2):

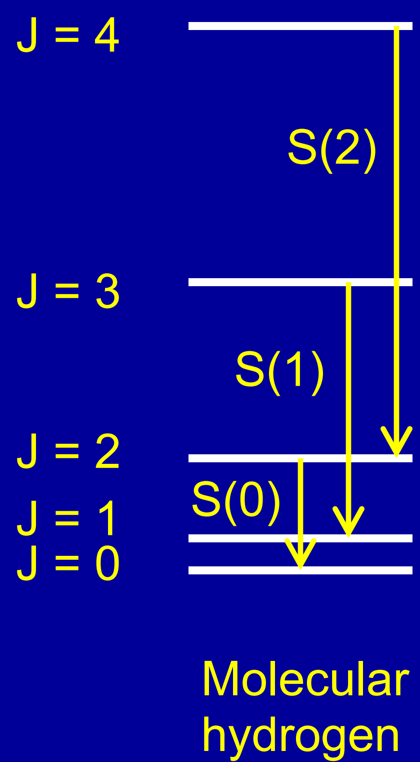
the rotational part of the wavefunction must be antisymmetric
➔ J is odd

For the total spin = 0 state (para-H_2):

the rotational part of the wavefunction must be symmetric
➔ J is even

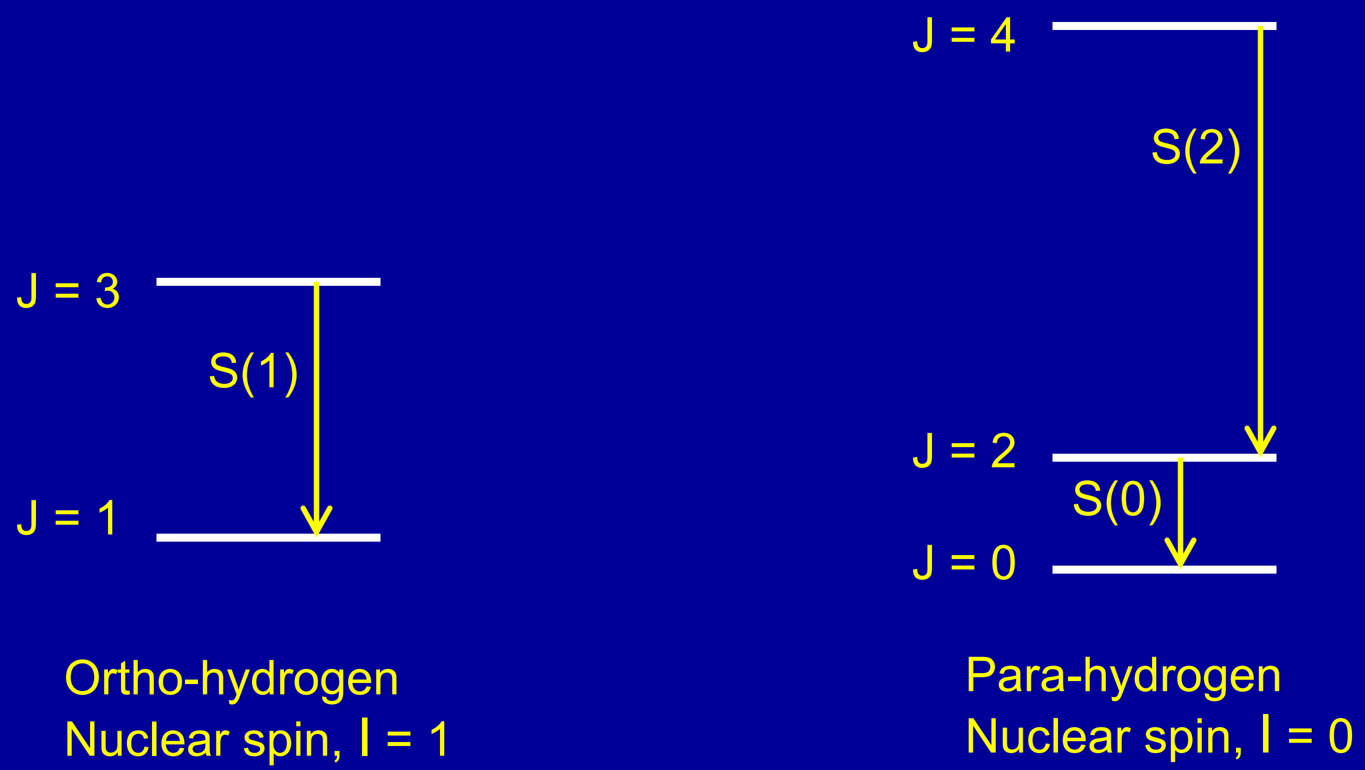
H_2 rotational structure

Absence of dipole moment ➔ $\Delta J = -2$ selection rule



H_2 rotational structure

Absence of dipole moment ➔ $\Delta J = -2$ selection rule



Equilibrium ortho-to-para ratio depends on temperature

High temperature:

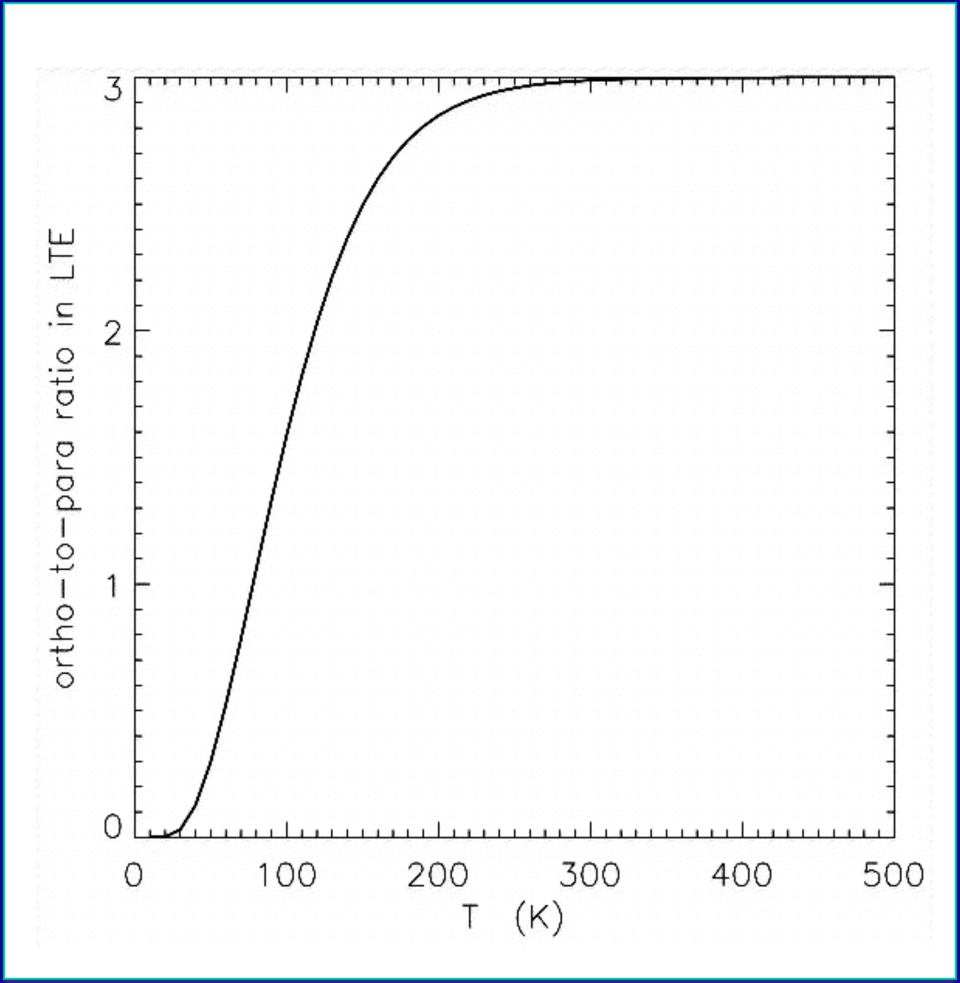
Ortho-H_2/para-H_2 = 3, the ratio of the nuclear spin degeneracies

Low temperature:

Ortho-H_2/para-H_2 = $n_{J=1}$ / $n_{J=0}$

= 9 exp (–171 K /T)

(less than 3 because lowest ortho-state is of higher energy)



Ortho-para conversion is extremely slow

Not only are $\Delta J = \pm 1$ transitions radiatively forbidden, they are negligible in non-reactive inelastic collisions

Reason: a change from even → odd J must be accompanied by a change in nuclear spin

Implication: ortho-to-para conversion is very slow

➔ may find non-equilibrium ortho-to-para ratios in H_2 that has recently changed temperature

A well known effect in the industrial production and storage of LH2

Straightforward refrigeration of H_2 leads to liquid H_2 with the ortho/para ratio initially "frozen in" at 3

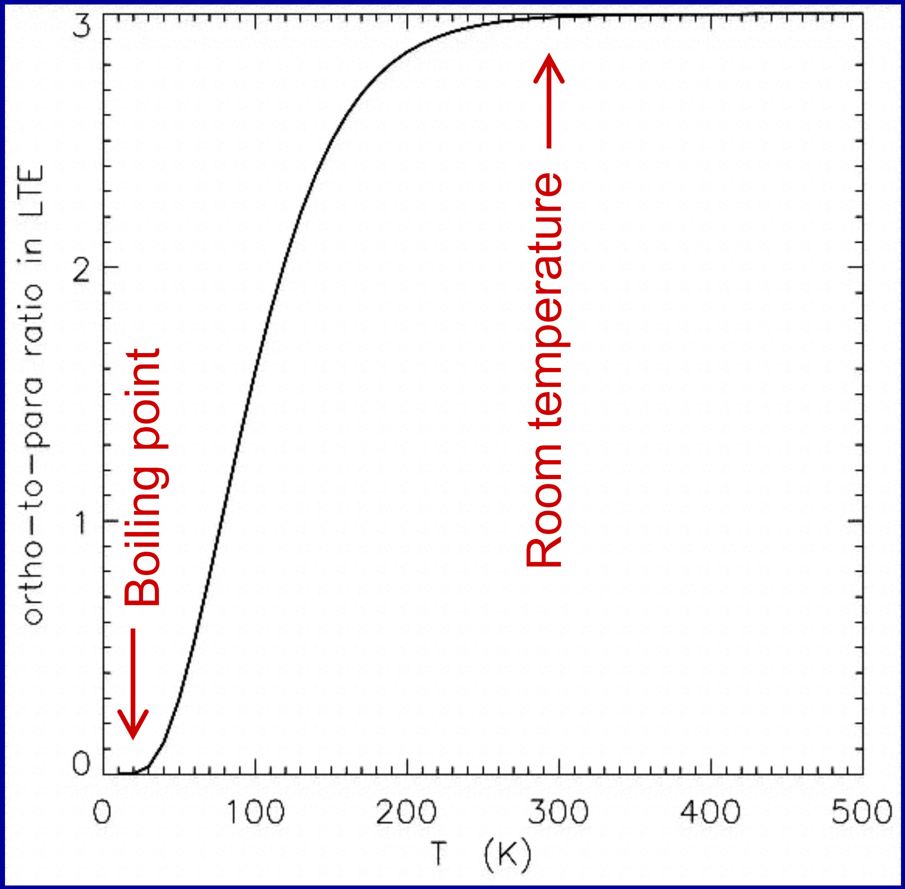
Ortho-to-para ratio in equilibrium

Room temperature:

Ortho-H_2/para-H_2 = 3

LH2 temperature:

Ortho-H_2/para-H_2 = 0.01



A well known effect in the industrial production and storage of LH2

Straightforward refrigeration of H_2 leads to liquid H_2 with the ortho/para ratio initially "frozen in" at 3

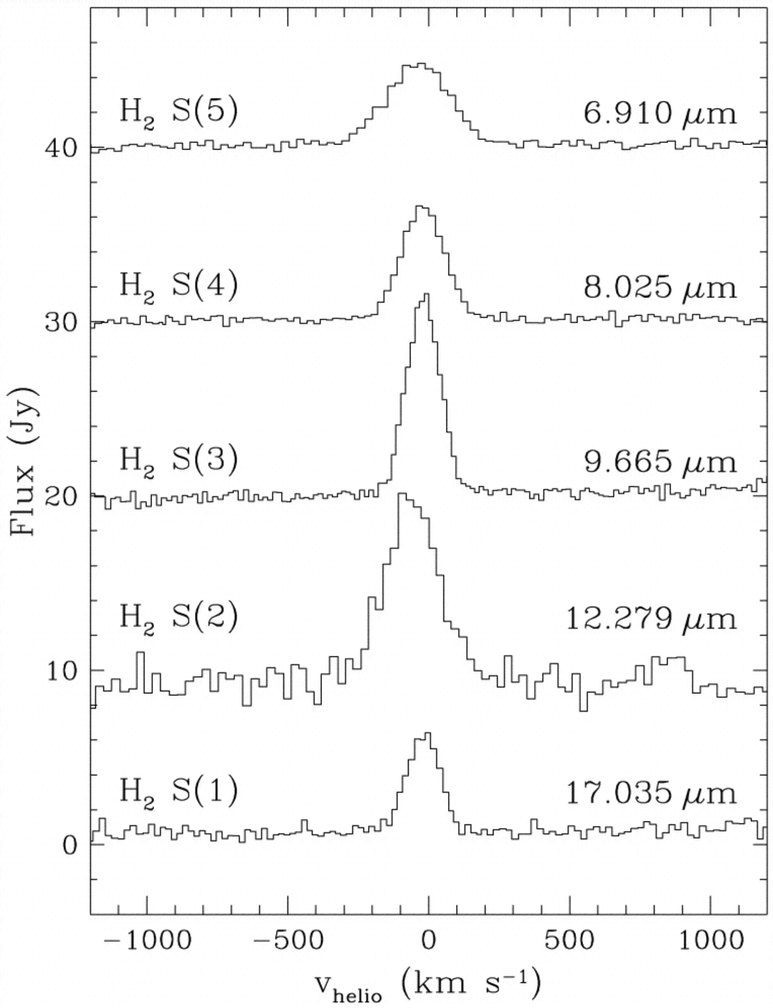
Ortho-para conversion proceeds slowly, with a timescale ~ 6.5 days, releasing heat as it occurs

A similar effect has also been observed with astrophysical H_2

Infrared Space Observatory (ISO/SWS) observations of HH54, a Herbig-Haro object in which molecular gas is shocked by a protostellar outflow

➔ detection of S(1) through S(5) pure rotational lines

(Neufeld et al. 1998, ApJL)



HH54 rotational diagram

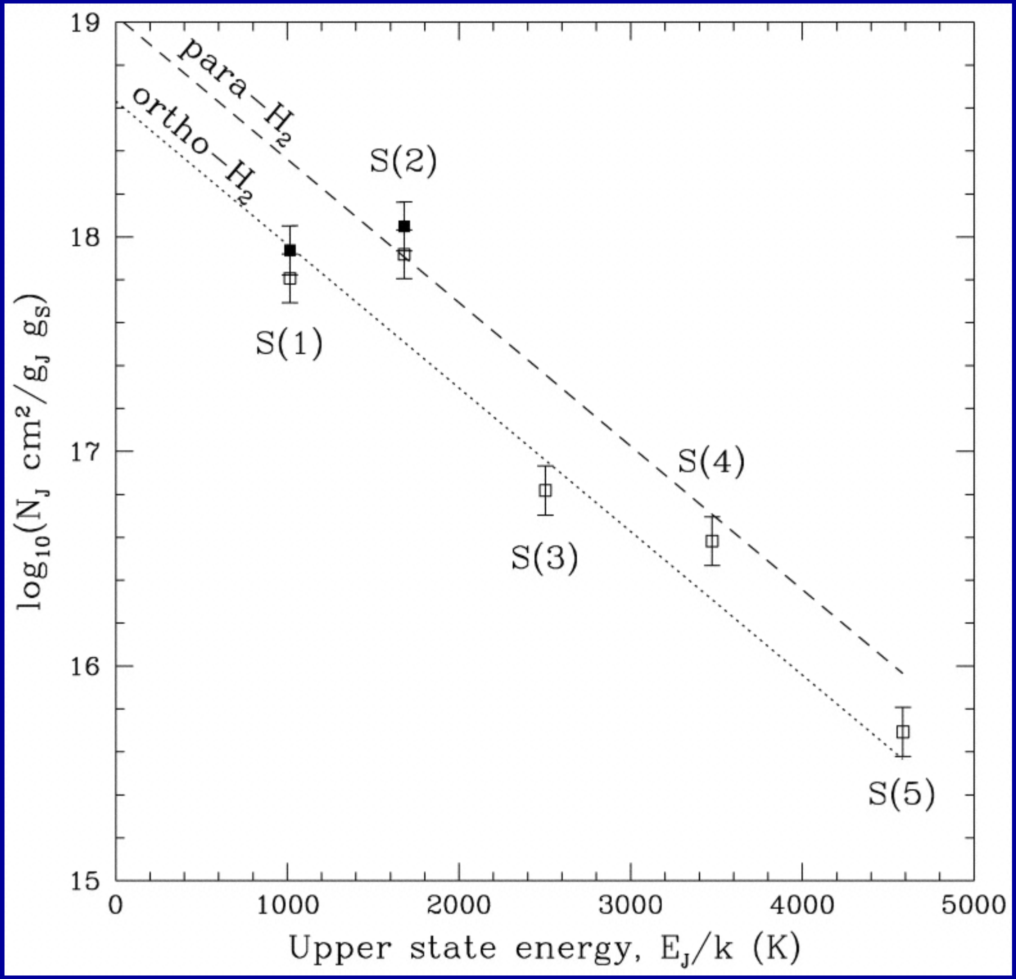
Zigzag behavior

➔ ortho-para ratio out of equilibrium

Slope ➔ T_{gas} = 650 K

Ortho-para ratio = 1.2

➔ T_{op} = 90 K



Shock heating suggested

- Shock waves heat gas temporarily: time spent hot is smaller than the ortho/para conversion time

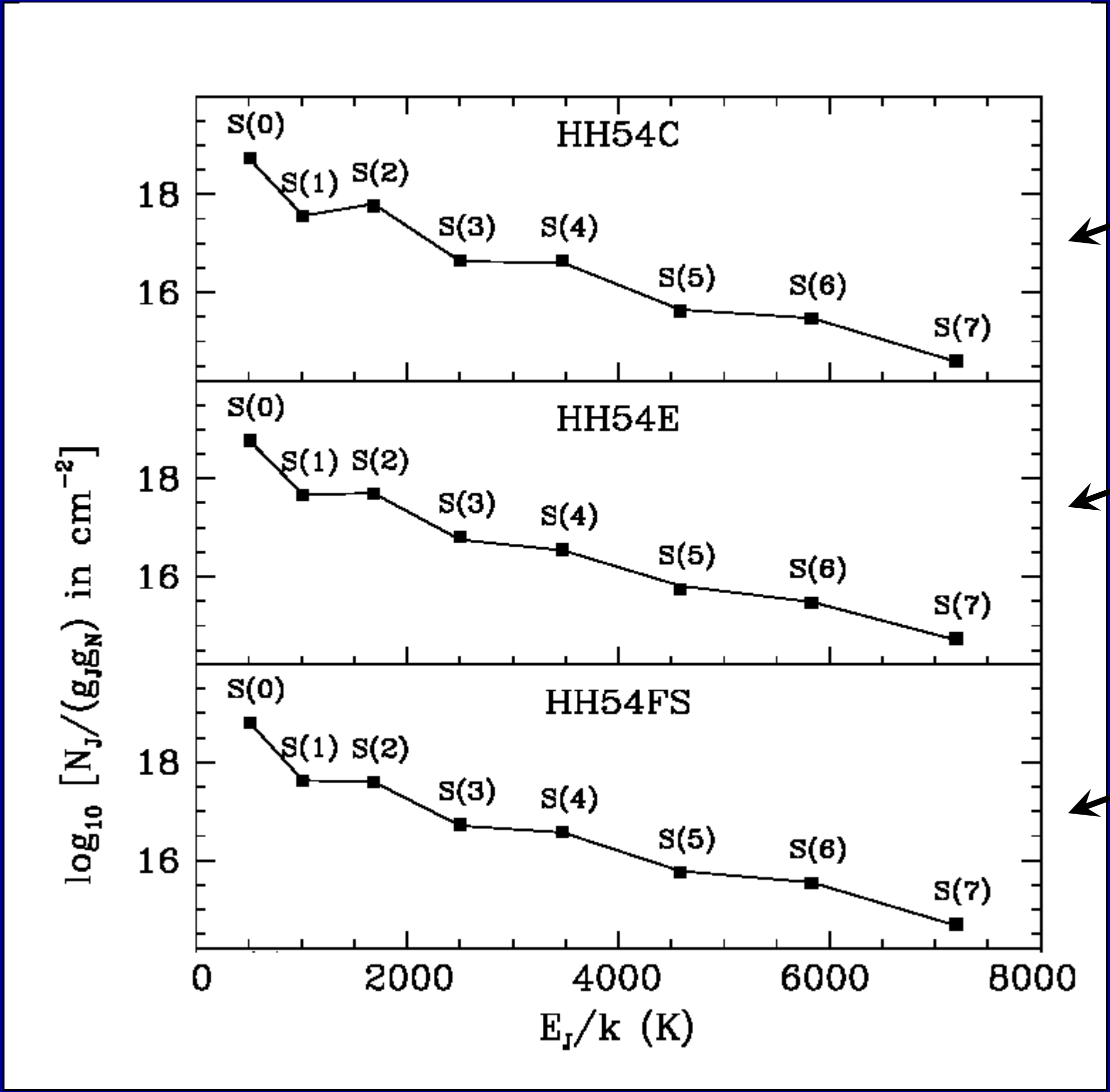
- Compared results with predictions based on detailed calculations of Timmerman (1996, ApJ)
  - Para-to-ortho conversion is dominated by reactive collisions

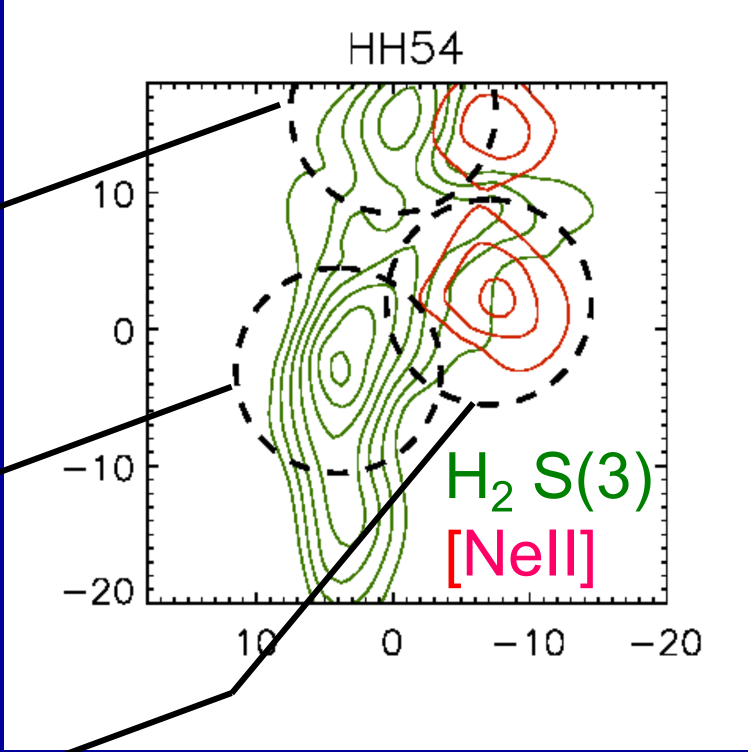
    $p - H_2 + H \rightarrow H + o - H_2$

    (activation energy barrier $\Delta E_A/k$ ~ 4000 K)

  - Ortho/para ratio in HH54 consistent with models for shocks with velocity 10 – 20 km/s

H_2 rotational diagrams for shock-heated gas in HH54 observed with Spitzer



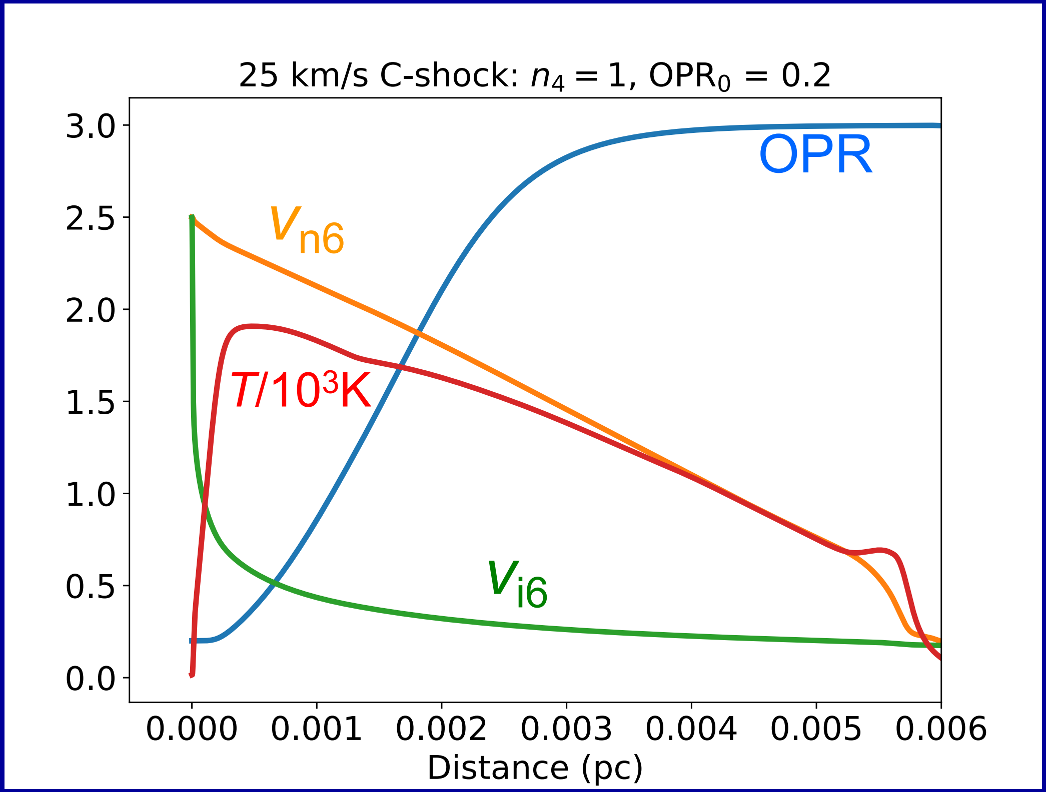


Fits to rotational diagrams

- Curvature → multiple temperatures present
  - We typically get good agreement with a two-component fit that invokes a warm component at T_W ~ 400 K and a hot component at T_H ~ 1000 K
  - Consistent with a mixture of shock velocities in the range 10 – 25 km/s
- Zigzag behavior
  - H_2 ortho-to-para ratio is smaller than 3: relic of an earlier time when the gas was cooler
  - Compelling evidence for non-equilibrium chemistry
  - Departures from equilibrium are greater for the lower temperature components
  - Para → ortho conversion more efficient in faster, hotter shocks

Can we actually see this para → ortho conversion taking place within a shock?

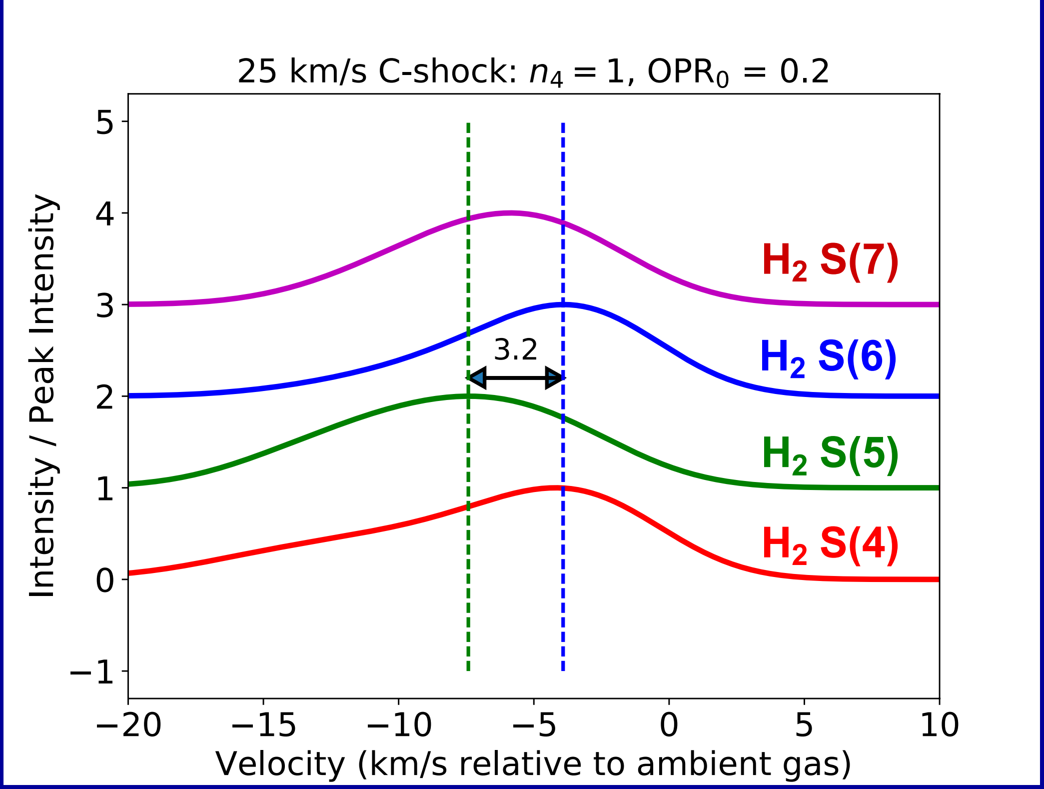
The linear scale is ~ (0.001/n_4) pc ~ (1/n_4) arcsec at 200 pc, where the preshock density of H nuclei = 10^4 n_4 cm^{-3}
(Should be detectable with JWST)



Pierre Lesaffre (Paris-Durham shock code)

Can we actually see this para → ortho conversion taking place within a shock?

But we might hope to see a frequency shift between the ortho- and para-H_2 lines



Pierre Lesaffre (Paris-Durham shock code)

Observations

Performed mid-Oct 2018 in Cycle 6 GO program

Total time: 10.5 hours spread over 4 flights

We observed four pure rotational emission lines of H_2

Two para-H_2 lines

S(4) (i.e. J = 6 – 4) at 8.2 μm

S(6) (i.e. J = 8 – 6) at 6.1 μm

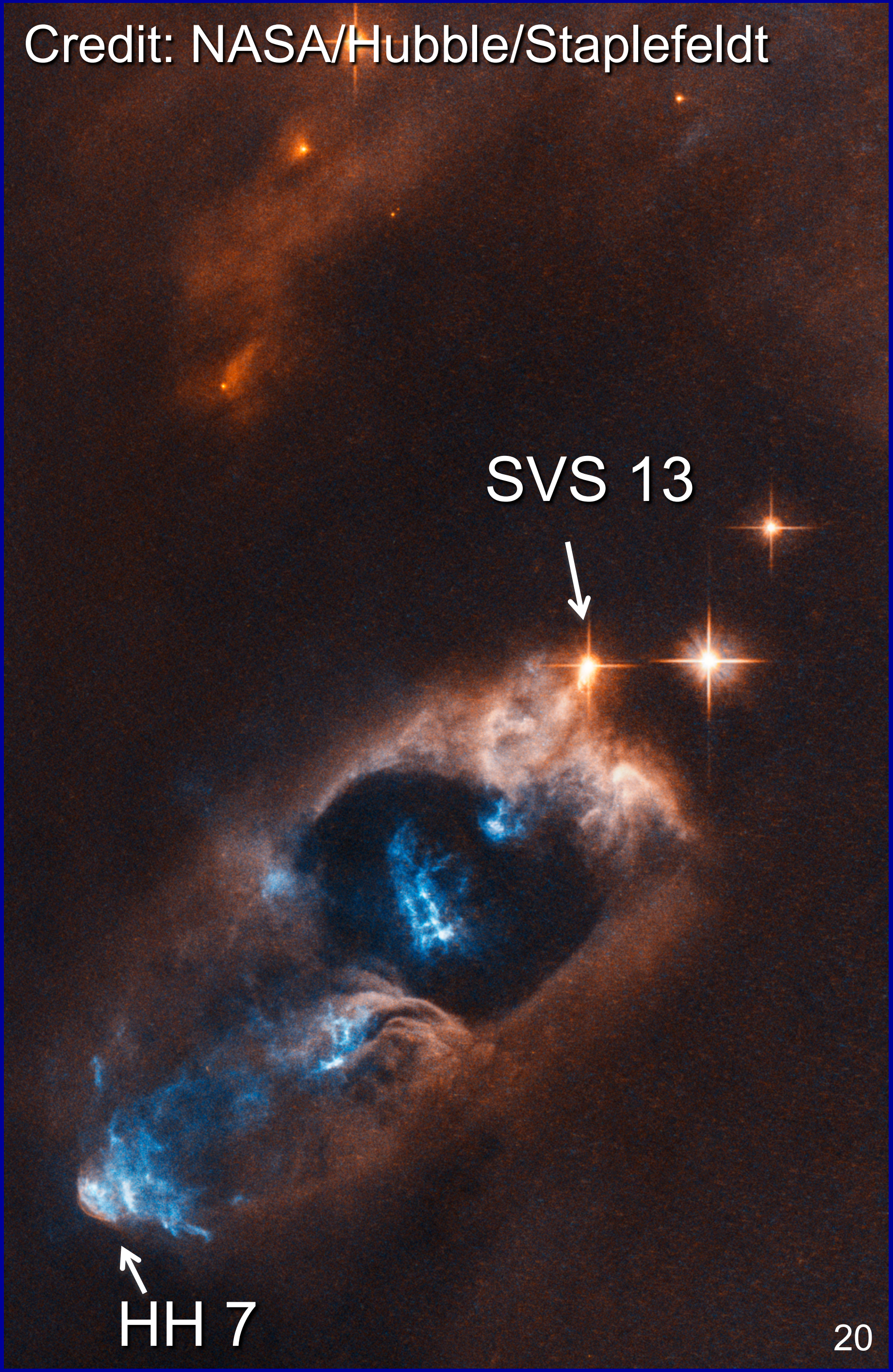
Two ortho-H_2 lines

S(5) (i.e. J = 7 – 5) at 6.9 μm

S(7) (i.e. J = 9 – 7) at 5.5 μm

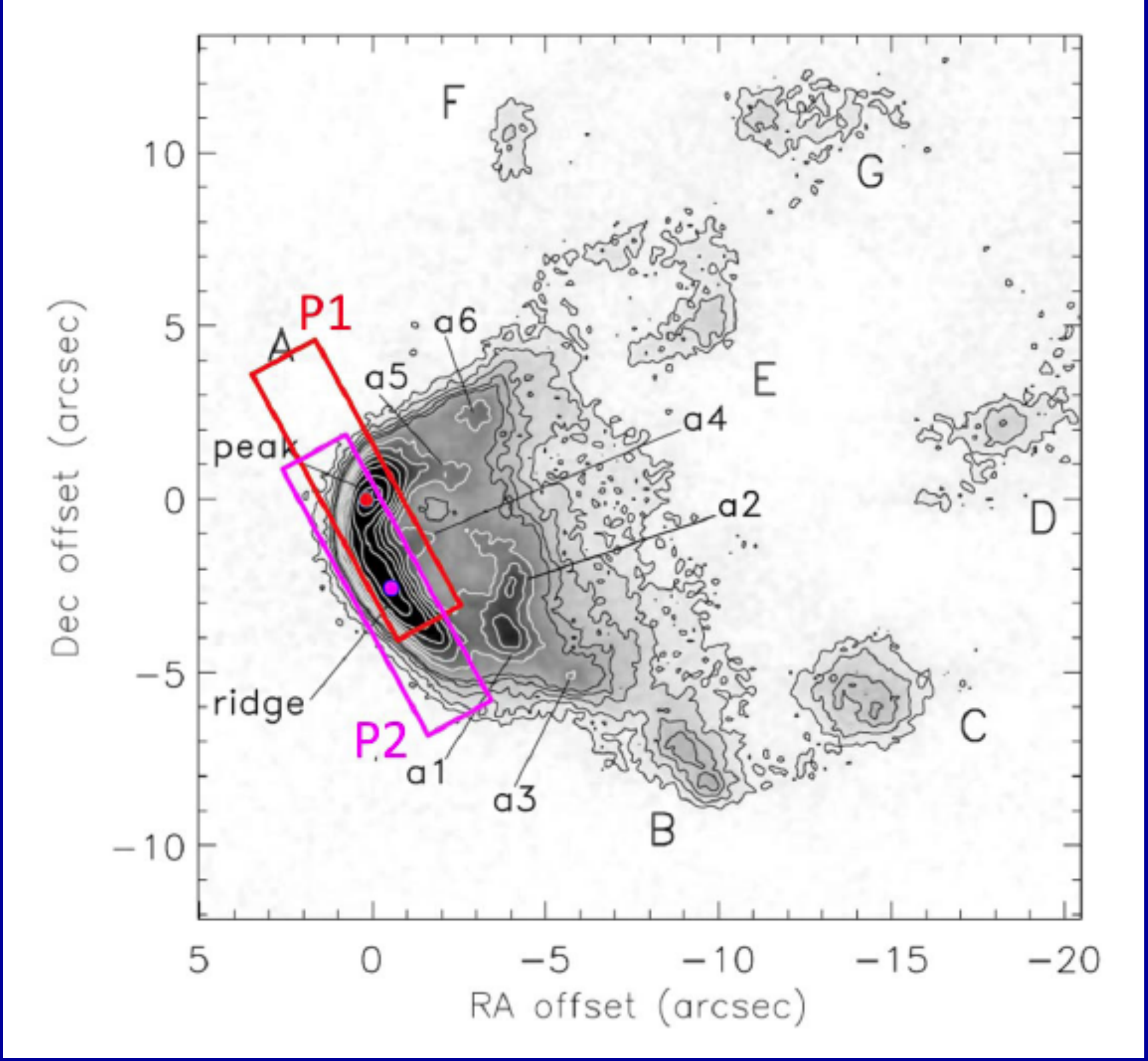
toward two positions in HH7

HH7: a bow shock driven by the jet from a YSO

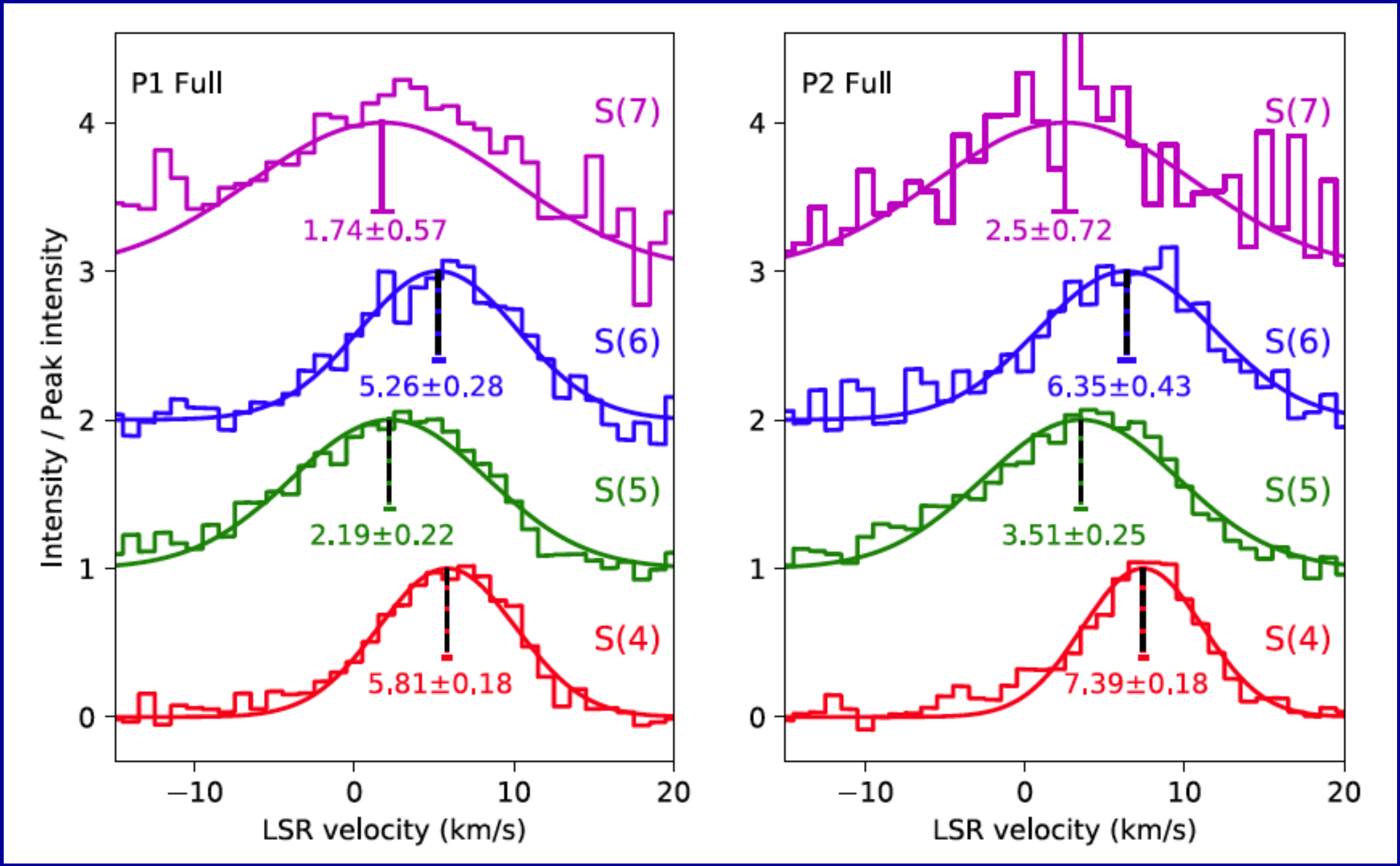


We used slit widths of 1.9 arcsec to achieve a spectral resolving power of 86,000

(equivalent to 3.5 km/s)



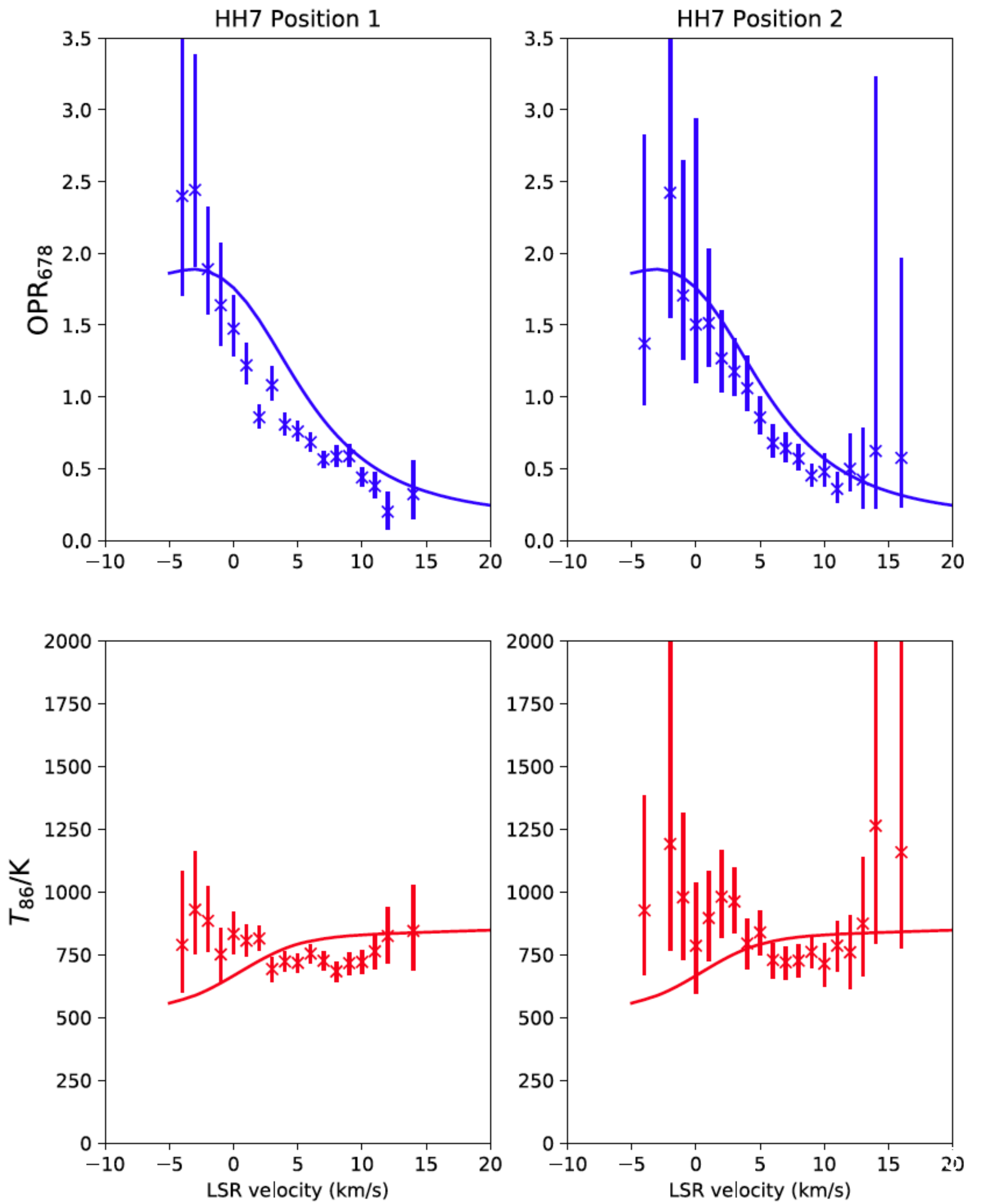
Observed spectra



Clear evidence for an ortho-para shift of 3 – 4 km/s

Relative strengths of S(4), S(5) and S(6) lines probe the ortho-to-para ratio and temperature

Can track para-ortho conversion through the shock



Conclusion

Zigzag rotational diagrams for the H_2 pure rotational lines observed from shocks provide the best example of interstellar chemistry that is out of equilibrium

With velocity-resolved observations, now possible for the first time with SOFIA/EXES, we can witness the return toward chemical equilibrium within the hot shocked gas

The ortho-para velocity shifts observed with EXES provide among the best evidence for ‘C’-type shocks in which the flow velocity varies continuously