CH_3^+: A New Tool for Studying the Enigma of Interstellar CH^+?

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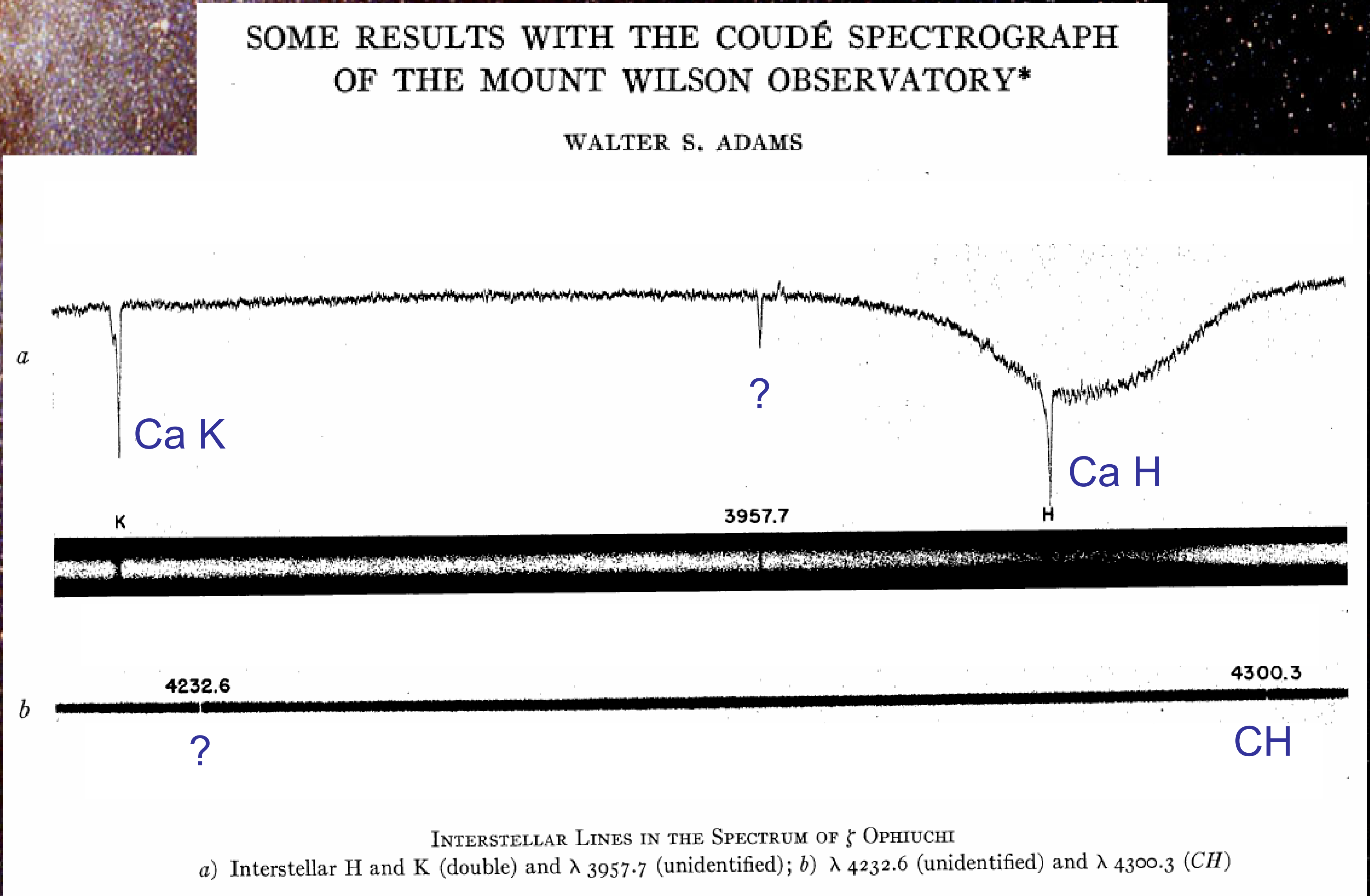
Discovery of CH^+



SOME RESULTS WITH THE COUDÉ SPECTROGRAPH OF THE MOUNT WILSON OBSERVATORY*

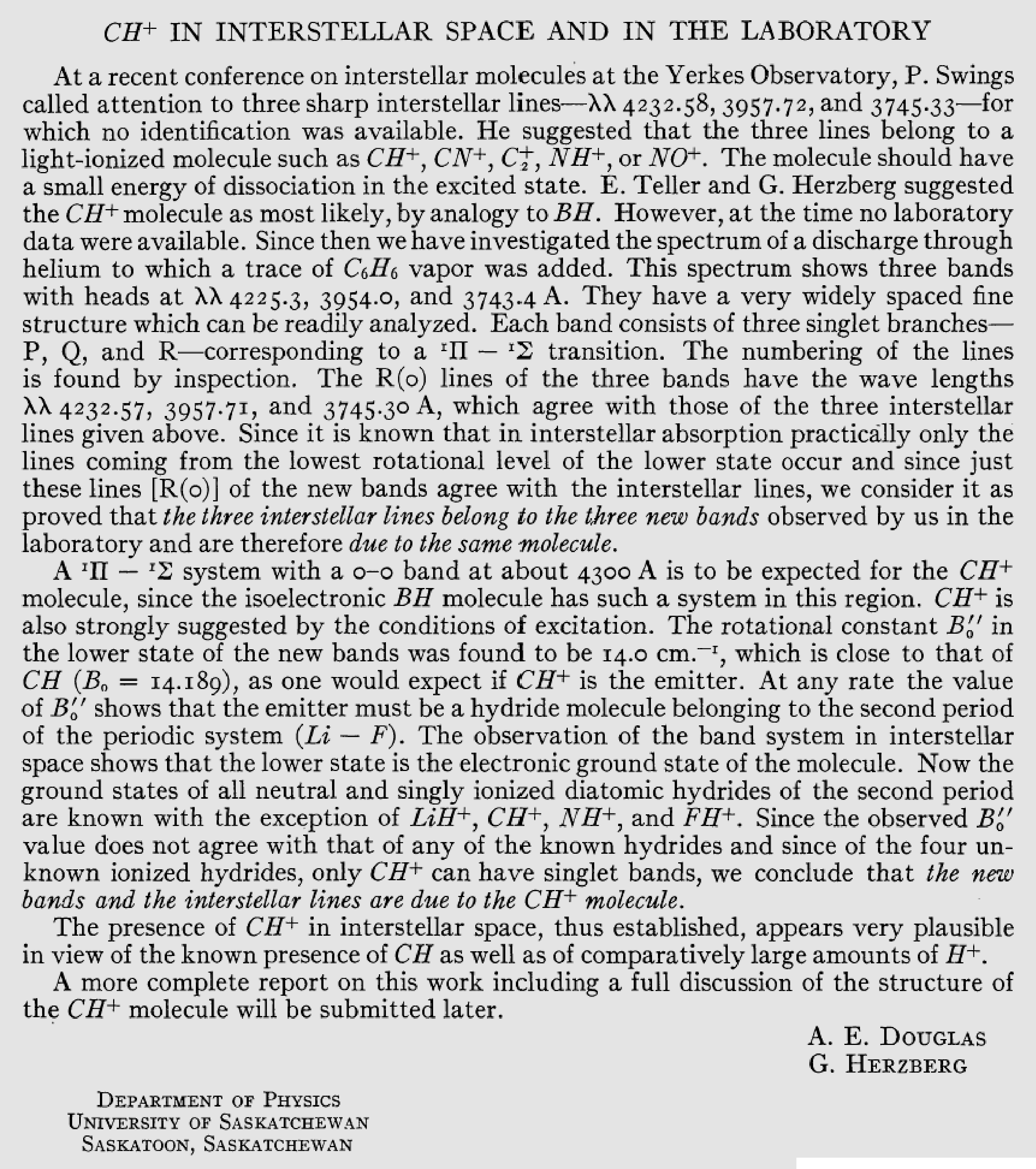
WALTER S. ADAMS

INTERSTELLAR LINES IN THE SPECTRUM OF ζ OPHIUCHI

a) Interstellar H and K (double) and λ 3957·7 (unidentified); *b*) λ 4232.6 (unidentified) and λ 4300.3 (*CH*)

Photo credit: allthesky.com

Adams, ApJ 93, 11 (1941)



CH^+ IN INTERSTELLAR SPACE AND IN THE LABORATORY

At a recent conference on interstellar molecules at the Yerkes Observatory, P. Swings called attention to three sharp interstellar lines—λλ 4232.58, 3957.72, and 3745.33—for which no identification was available. He suggested that the three lines belong to a light-ionized molecule such as CH^+, CN^+, C_2^+, NH^+, or NO^+. The molecule should have a small energy of dissociation in the excited state. E. Teller and G. Herzberg suggested the CH^+ molecule as most likely, by analogy to BH. However, at the time no laboratory data were available. Since then we have investigated the spectrum of a discharge through helium to which a trace of C_6H_6 vapor was added. This spectrum shows three bands with heads at λλ 4225.3, 3954.0, and 3743.4 A. They have a very widely spaced fine structure which can be readily analyzed. Each band consists of three singlet branches—P, Q, and R—corresponding to a $^1\Pi - {}^1\Sigma$ transition. The numbering of the lines is found by inspection. The R(0) lines of the three bands have the wave lengths λλ 4232.57, 3957.71, and 3745.30 A, which agree with those of the three interstellar lines given above. Since it is known that in interstellar absorption practically only the lines coming from the lowest rotational level of the lower state occur and since just these lines [R(0)] of the new bands agree with the interstellar lines, we consider it as proved that *the three interstellar lines belong to the three new bands* observed by us in the laboratory and are therefore *due to the same molecule.*

A $^1\Pi - {}^1\Sigma$ system with a 0–0 band at about 4300 A is to be expected for the CH^+ molecule, since the isoelectronic BH molecule has such a system in this region. CH^+ is also strongly suggested by the conditions of excitation. The rotational constant B_0'' in the lower state of the new bands was found to be 14.0 cm.$^{-1}$, which is close to that of CH ($B_0 = 14.189$), as one would expect if CH^+ is the emitter. At any rate the value of B_0'' shows that the emitter must be a hydride molecule belonging to the second period of the periodic system ($Li - F$). The observation of the band system in interstellar space shows that the lower state is the electronic ground state of the molecule. Now the ground states of all neutral and singly ionized diatomic hydrides of the second period are known with the exception of LiH^+, CH^+, NH^+, and FH^+. Since the observed B_0'' value does not agree with that of any of the known hydrides and since of the four unknown ionized hydrides, only CH^+ can have singlet bands, we conclude that *the new bands and the interstellar lines are due to the CH^+ molecule.*

The presence of CH^+ in interstellar space, thus established, appears very plausible in view of the known presence of CH as well as of comparatively large amounts of H^+.

A more complete report on this work including a full discussion of the structure of the CH^+ molecule will be submitted later.

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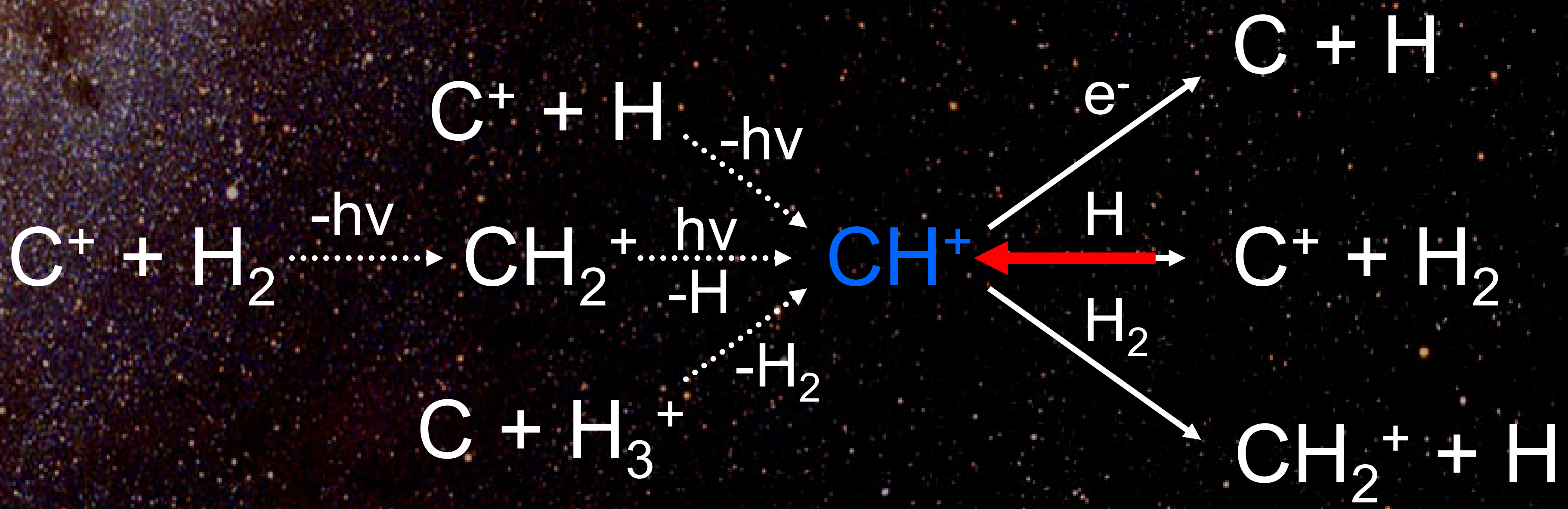
Douglas & Herzberg, ApJ 94, 381 (1941)

Enigma of CH^+



$C^+ + H_2 \xrightarrow{-hv} CH_2^+ \xrightarrow[-H]{hv} CH^+$

$C^+ + H \xrightarrow{-hv} CH^+$

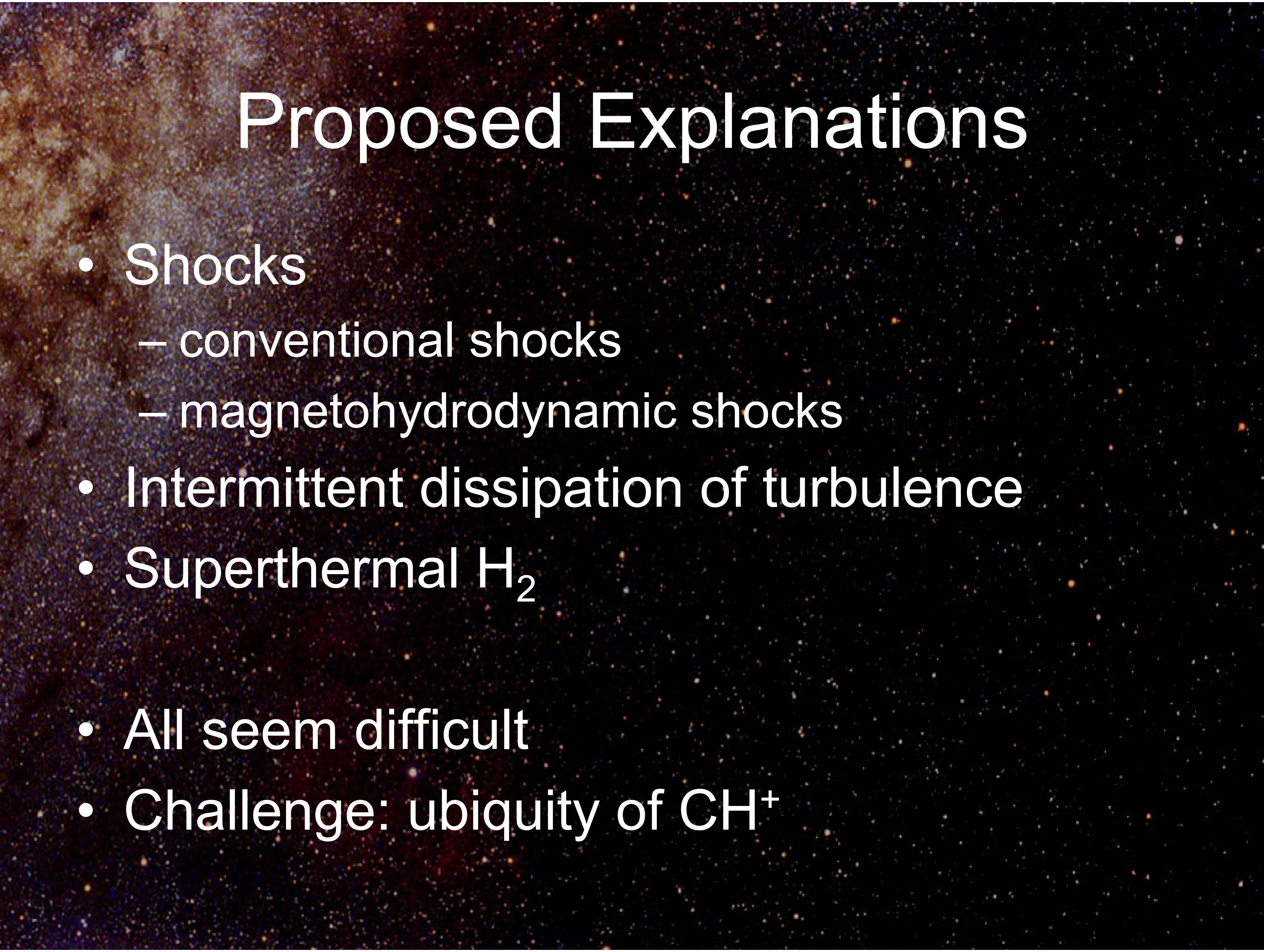
$C + H_3^+ \xrightarrow{-H_2} CH^+$

$CH^+ \xrightarrow{e^-} C + H$

$CH^+ \overset{H}{\rightleftarrows} C^+ + H_2$

$CH^+ \xrightarrow{H_2} CH_2^+ + H$

endothermic ~4640 K

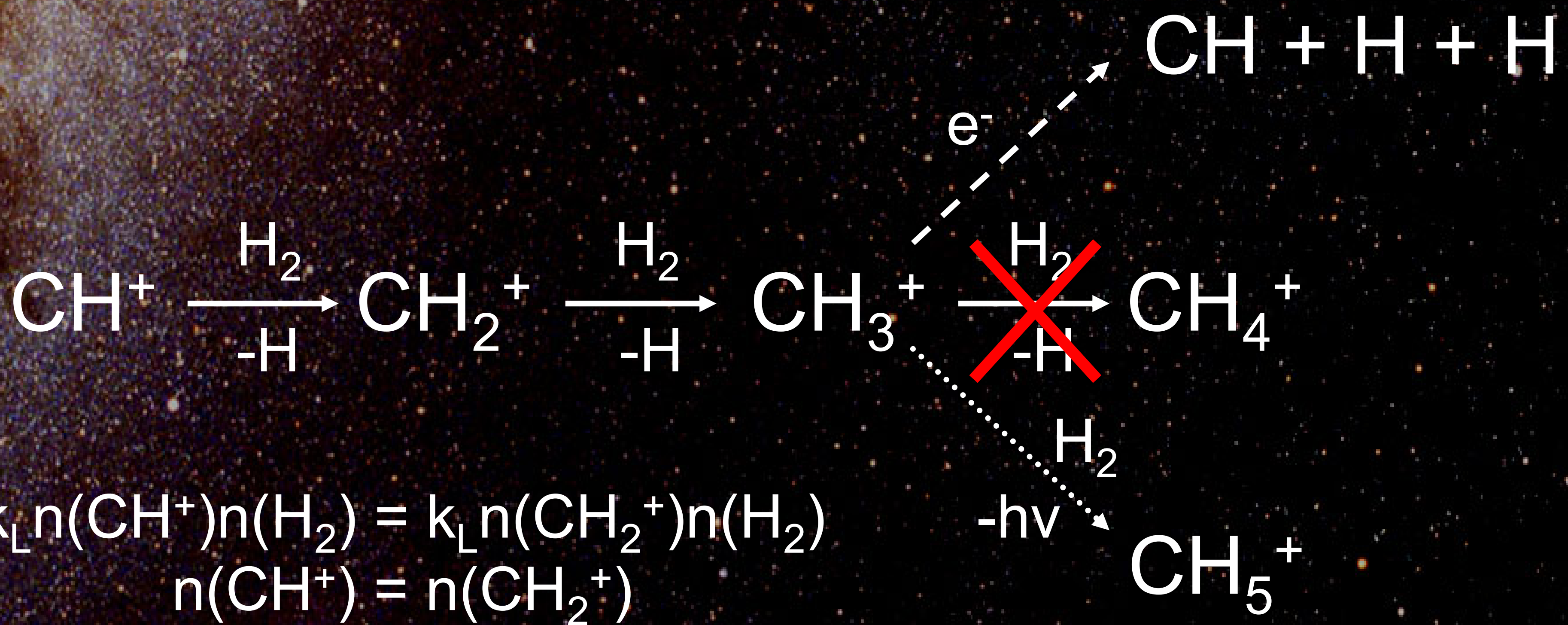


Proposed Explanations

- Shocks
  - conventional shocks
  - magnetohydrodynamic shocks
- Intermittent dissipation of turbulence
- Superthermal H_2

- All seem difficult
- Challenge: ubiquity of CH^+

CH^+ Chemistry



$$CH^+ \xrightarrow[-H]{H_2} CH_2^+ \xrightarrow[-H]{H_2} CH_3^+ \cancel{\xrightarrow[-H]{H_2}} CH_4^+$$

$$CH_3^+ \xrightarrow{e^-} CH + H + H$$

$$CH_3^+ \xrightarrow[-h\nu]{H_2} CH_5^+$$

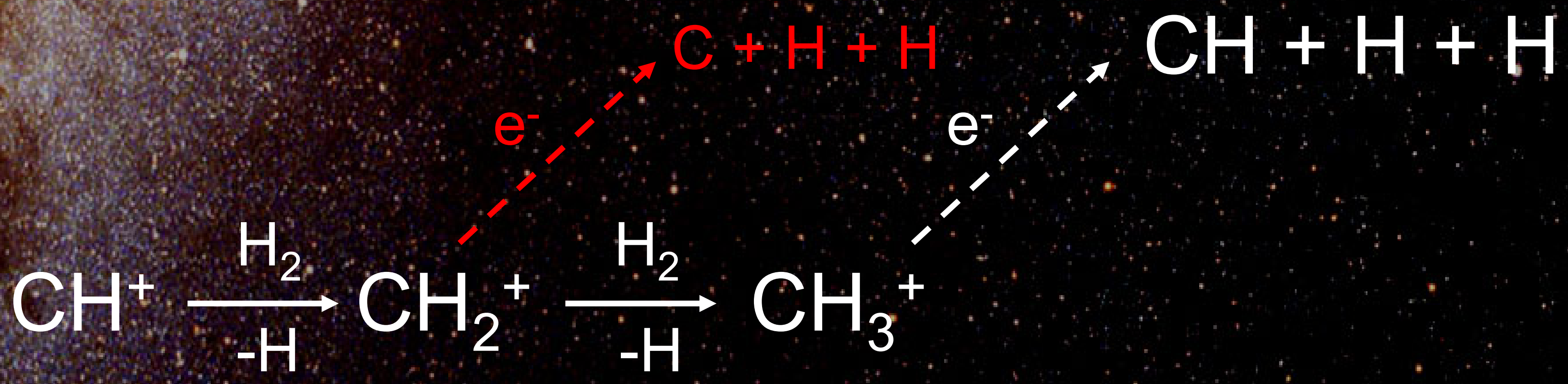
$$k_L n(CH^+) n(H_2) = k_L n(CH_2^+) n(H_2)$$

$$n(CH^+) = n(CH_2^+)$$

$$k_L n(CH_2^+) n(H_2) = k_e n(CH_3^+) n(e^-)$$

$$\frac{n(CH_3^+)}{n(CH^+)} = \frac{n(CH_3^+)}{n(CH_2^+)} = \frac{k_L}{k_e} \frac{n(H_2)}{n(e^-)} \sim \frac{10^{-9}}{10^{-7}} \cdot 10^4 \sim 10^2$$

A Less Rosy Scenario



$$CH^+ \xrightarrow[-H]{H_2} CH_2^+ \xrightarrow[-H]{H_2} CH_3^+$$

$$CH_2^+ \xrightarrow{e^-} C + H + H$$

$$CH_3^+ \xrightarrow{e^-} CH + H + H$$

- Dissociative recombination of CH_2^+ is fast
  - – especially at low T
- Hydrogen may not be fully molecular

$$f = \frac{2n(H_2)}{n(H) + 2n(H_2)}$$

Steady-State CH_3^+

$$\frac{n(CH_3^+)}{n(CH^+)} = \frac{f^2 k_1}{2k_4 z\,(f + 2zk_3/k_2)}$$

T \ f	0.03	0.1	0.3	1.0
30	0.01	0.08	0.52	2.96
100	0.03	0.22	1.21	5.69
300	0.07	0.51	2.35	9.65
1000	0.19	1.13	4.41	16.46

$n_H \equiv n(H) + 2n(H_2)$

$f \equiv 2n(H_2) / n_H$

$z \equiv n(e^-) / n_H$

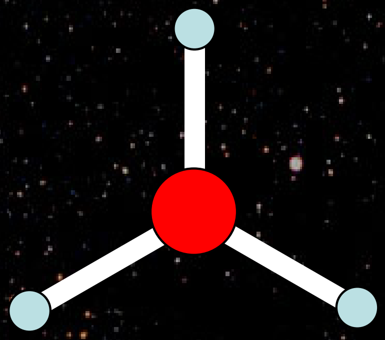
$CH^+ + H_2 \rightarrow CH_2^+ + H$ $k_1 = 1.2\times10^{-9}$

$CH_2^+ + H_2 \rightarrow CH_3^+ + H$ $k_2 = 1.6\times10^{-9}$

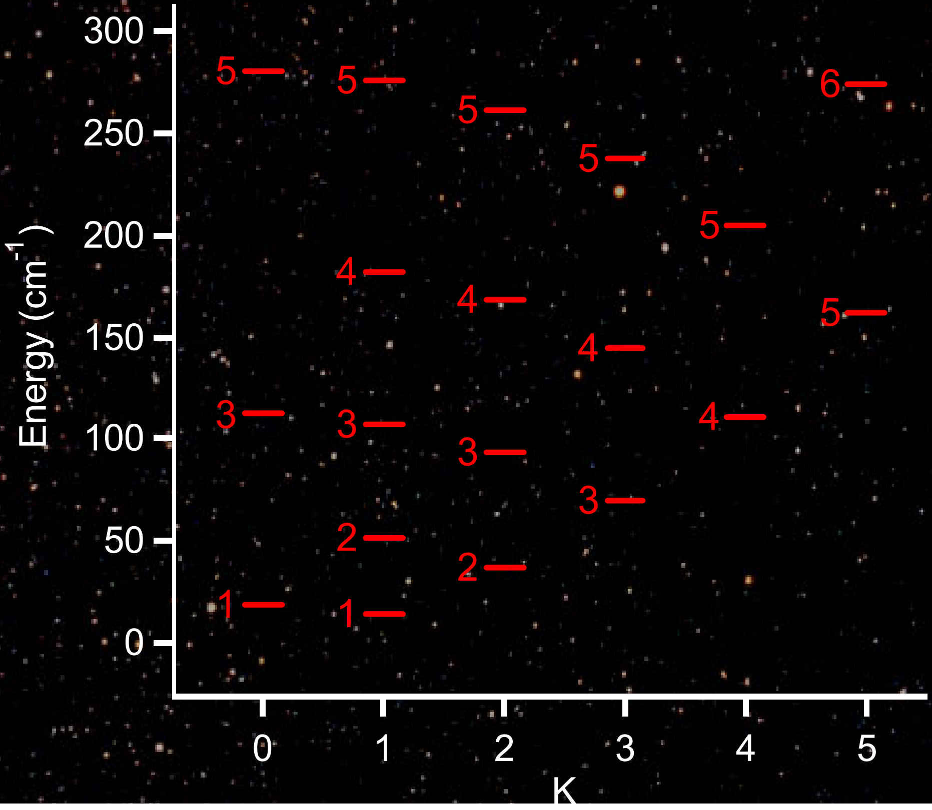
$CH_2^+ + e^- \rightarrow$ (products) $k_3 = 6.3\times10^{-7}\,(T/300)^{-0.6}$

$CH_3^+ + e^- \rightarrow$ (products) $k_4 = 4\times10^{-7}\,(T/300)^{-0.4}$

Spectroscopy of CH_3^+



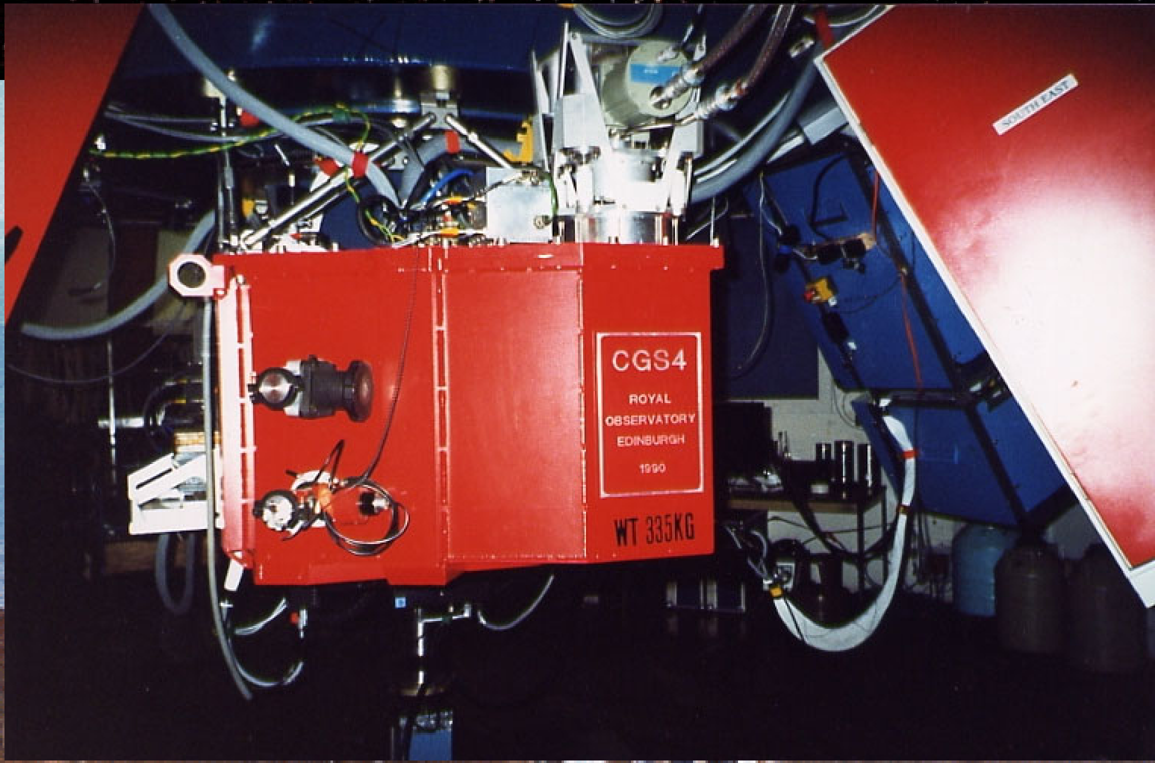
- No permanent dipole moment
- No known electronic spectrum
- ν_3 fundamental band ~3100 cm^{-1}
  - – measured by Oka group
    - ${}^rR(1,0)$ 3139.49 cm^{-1}
    - ${}^rR(1,1)$ 3129.13 cm^{-1}
    - ${}^rR(2,2)$ 3136.99 cm^{-1}



Crofton et al., JCP 83, 3702 (1985)

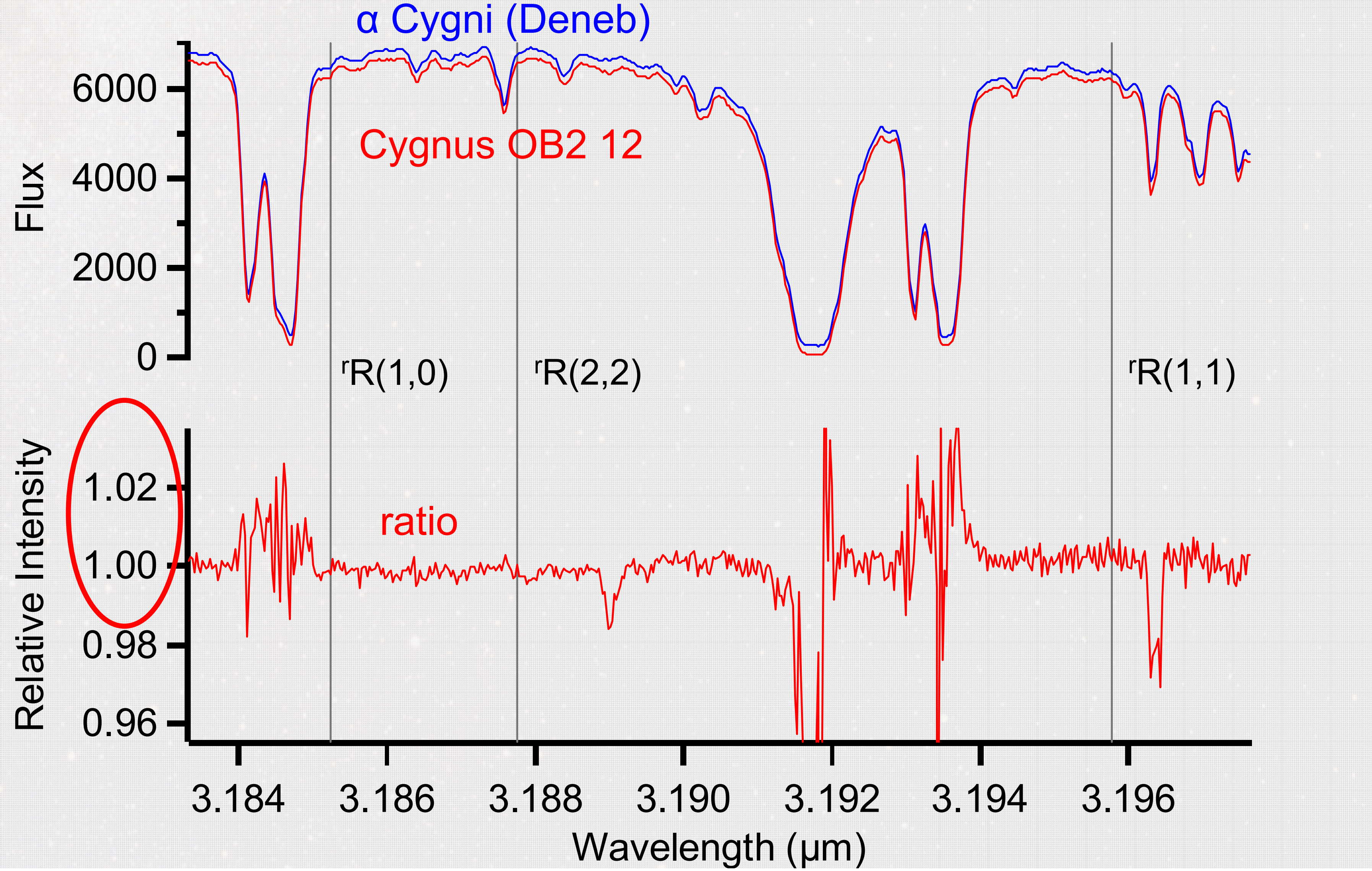
Observations

- Nov 19-20, 1999
- Targets:
  - Cygnus OB2 12
  - 1 Cas, σ Cas
  - 20 Tau, 23 Tau
  - ξ Per



Search for CH_3^+

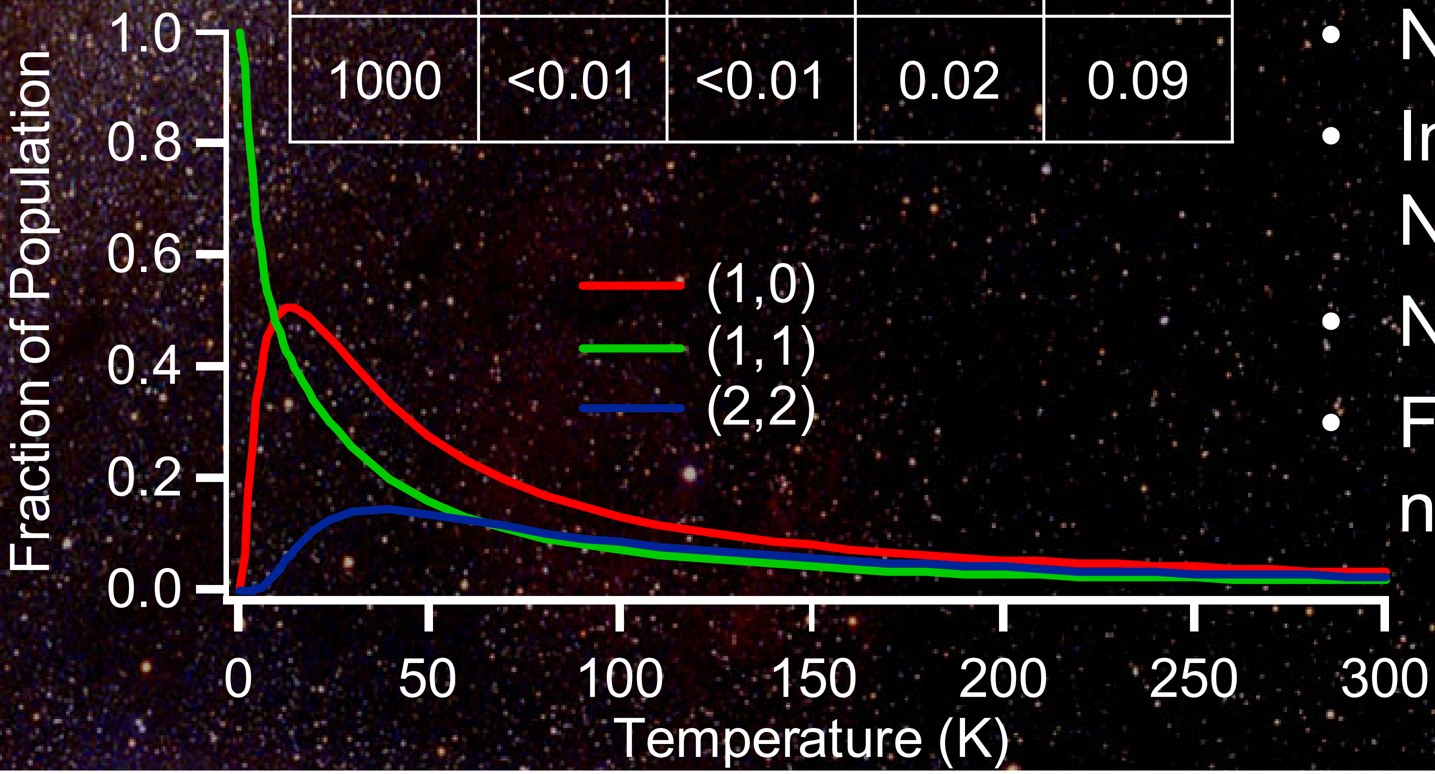
$^rR(1,0) \rightarrow N(1,0) \lesssim 6 \times 10^{13}\ \text{cm}^{-2}$



Rotational Distribution

T f	0.03	0.1	0.3	1.0
30	<0.01	0.03	0.21	1.21
100	<0.01	0.03	0.16	0.75
300	<0.01	0.02	0.07	0.30
1000	<0.01	<0.01	0.02	0.09

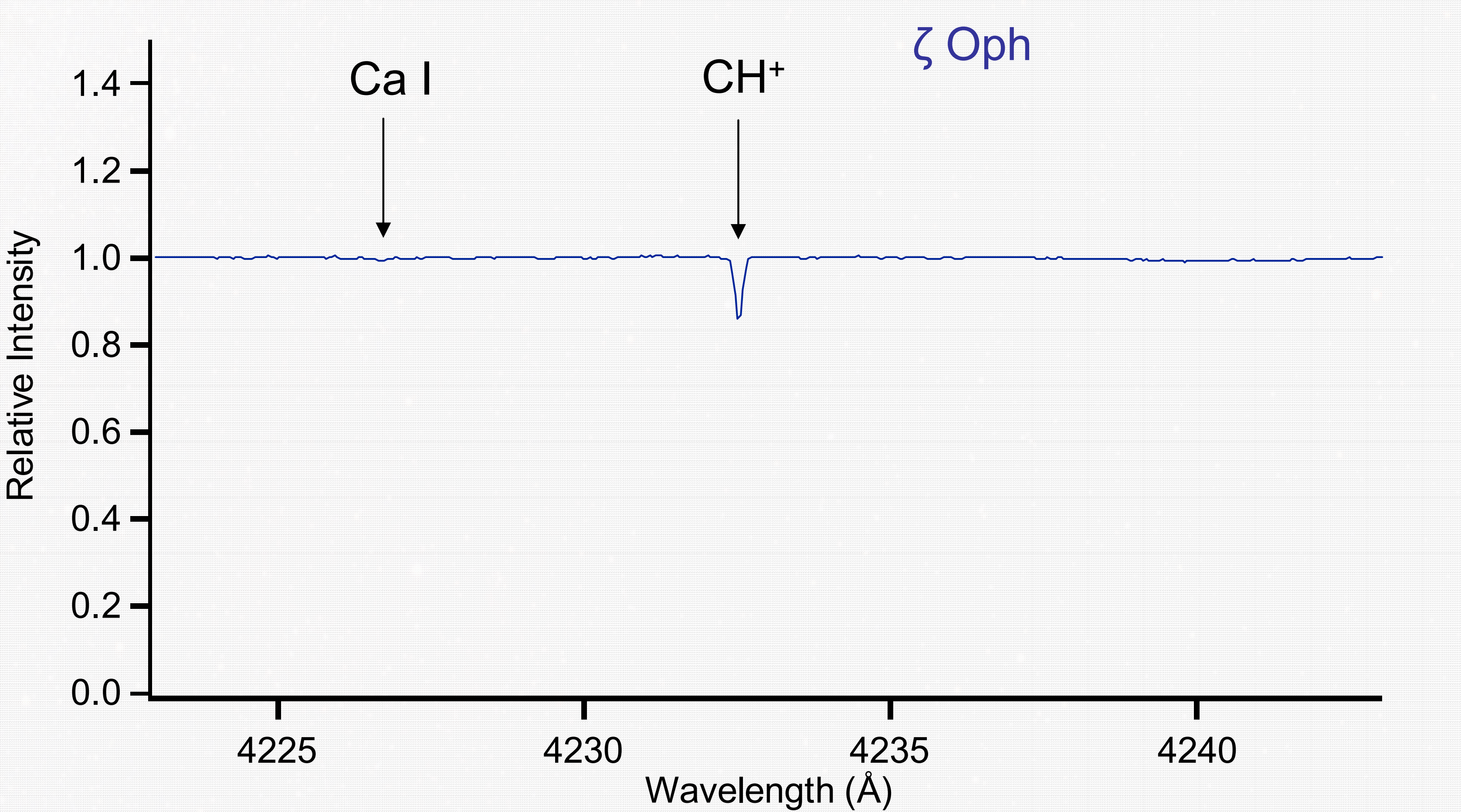
$$\frac{n(1,0)}{n(CH^+)}$$



- $N(1,0) \lesssim 6 \times 10^{13}$ cm^{-2}
- In most sightlines, $N(CH^+) \sim 3\times10^{13}$ cm^{-2}
- $N(1,0)/N(CH^+) \lesssim 2$!
- For meaningful limit, need higher $N(CH^+)$

CH^+ Spectra

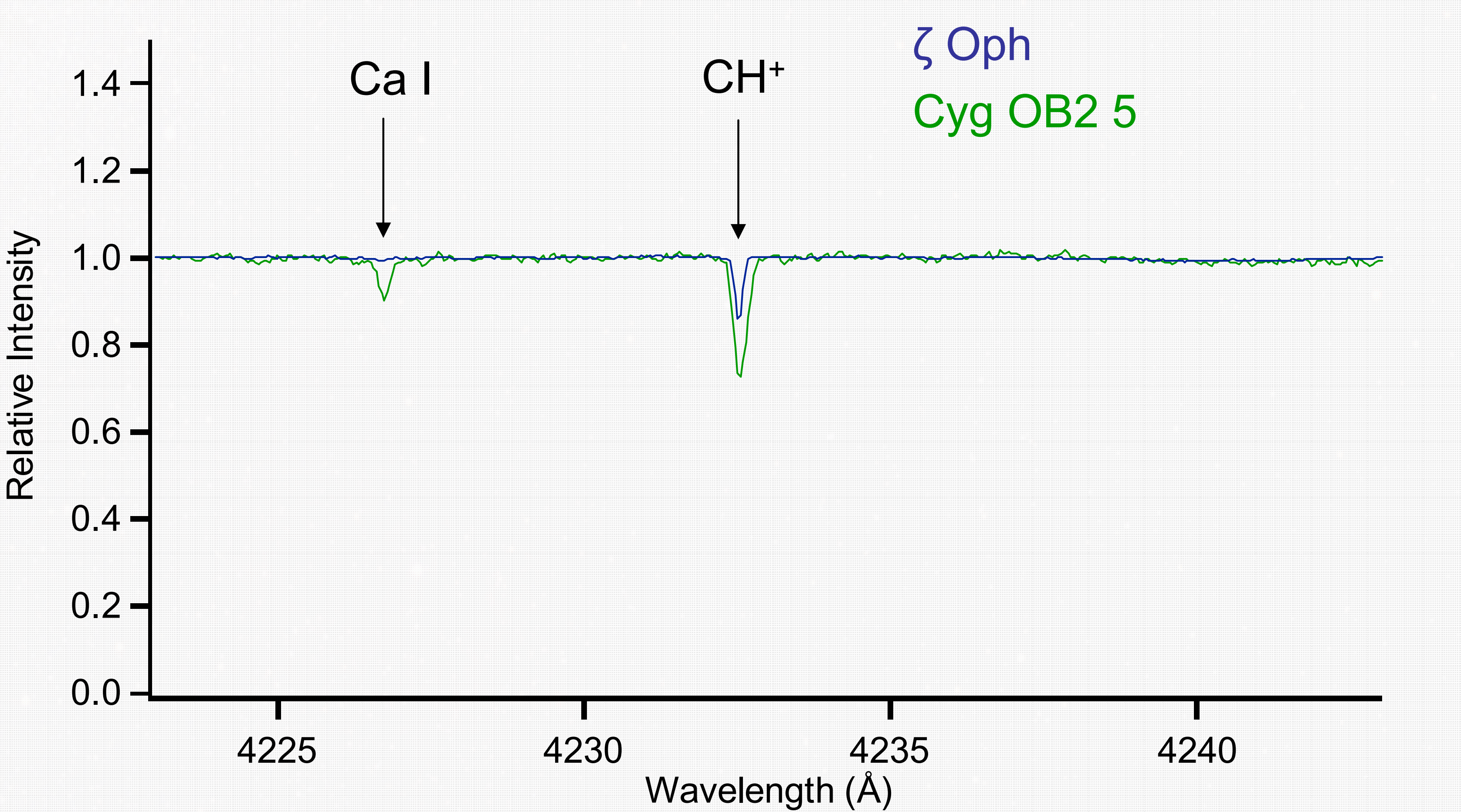
- ζ Oph $N(CH^+) = 3.4 \times 10^{13}$ cm^{-2} $E_{B-V} = 0.3$



Data from APO DIB Group (York et al.)

CH^+ Spectra

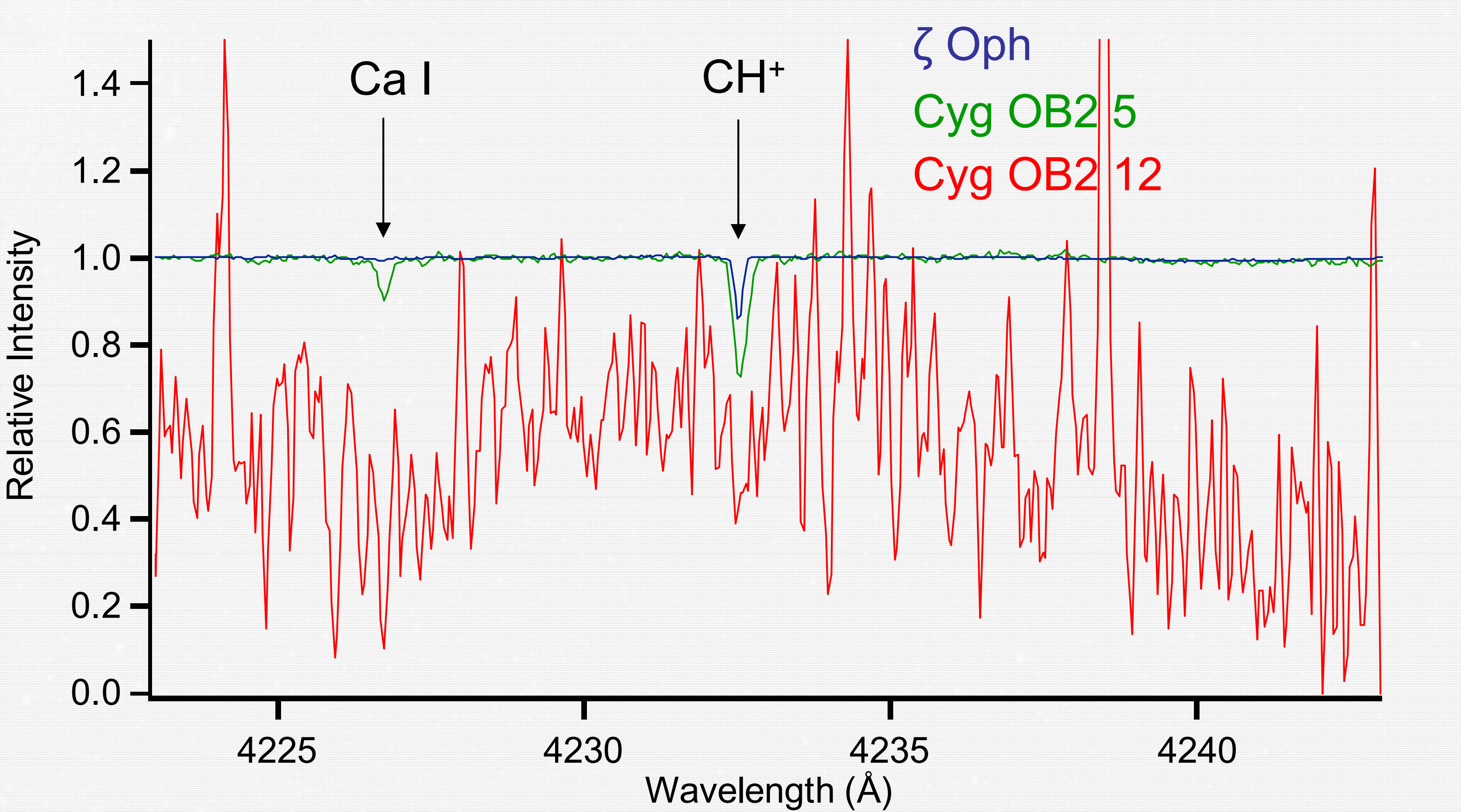
- ζ Oph $N(CH^+) = 3.4 \times 10^{13}\ cm^{-2}$ $E_{B-V} = 0.3$
- Cyg OB2 5 $N(CH^+) > 1.1 \times 10^{14}\ cm^{-2}$ $E_{B-V} = 2.0$



Data from APO DIB Group (York et al.)

CH^+ Spectra

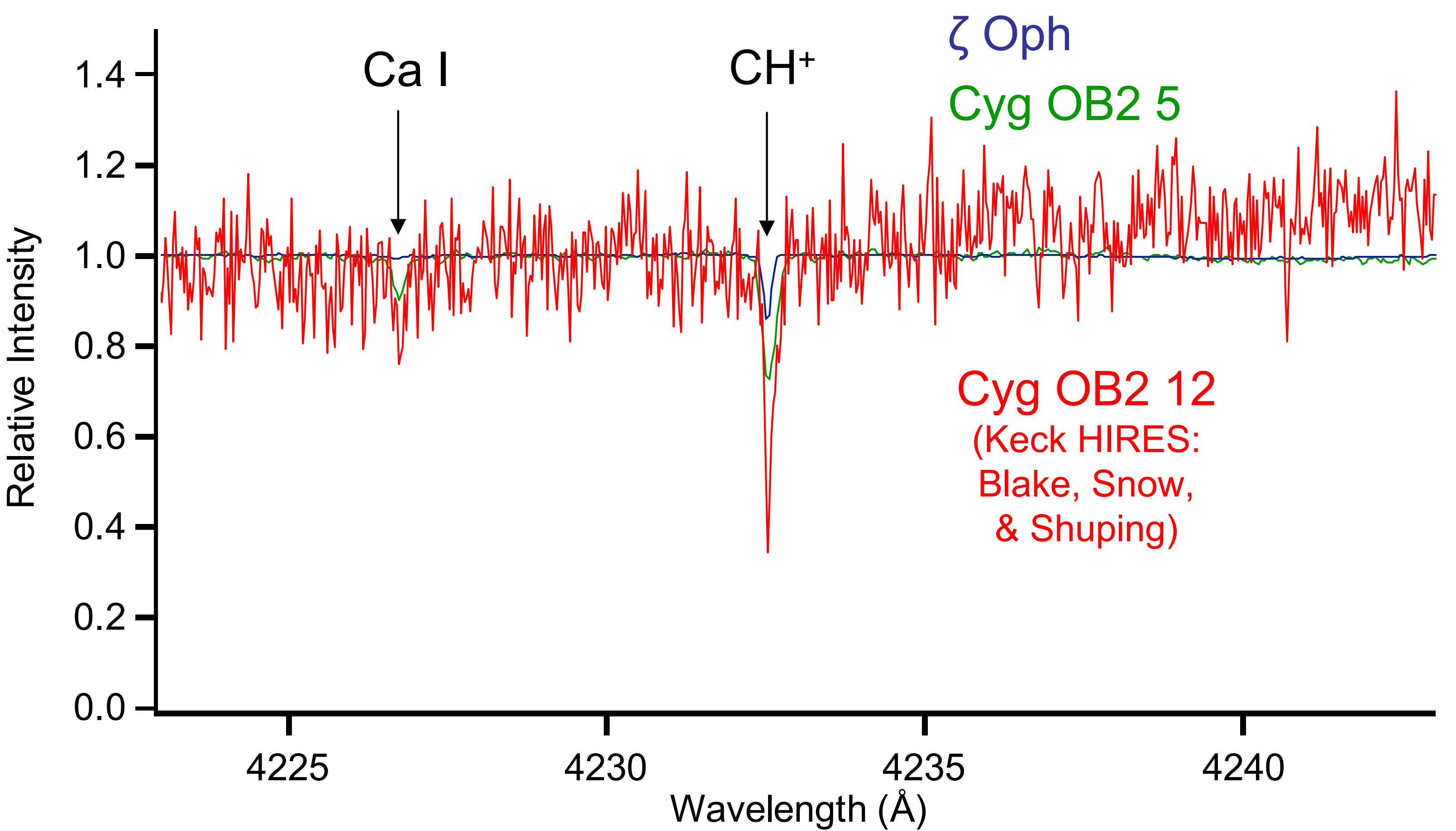
•	ζ Oph	$N(CH^+) = 3.4 \times 10^{13}\ cm^{-2}$	$E_{B-V} = 0.3$
•	Cyg OB2 5	$N(CH^+) > 1.1 \times 10^{14}\ cm^{-2}$	$E_{B-V} = 2.0$
•	Cyg OB2 12	$N(CH^+) = ?$ [B=14.4]	$E_{B-V} = 3.3$



Data from APO DIB Group (York et al.)

CH^+ Spectra

• ζ Oph	$N(CH^+) = 3.4 \times 10^{13}$ cm^{-2}	$E_{B-V} = 0.3$
• Cyg OB2 5	$N(CH^+) > 1.1 \times 10^{14}$ cm^{-2}	$E_{B-V} = 2.0$
• Cyg OB2 12	$N(CH^+) > 1.6 \times 10^{14}$ cm^{-2}	$E_{B-V} = 3.3$



Data
from
APO
DIB
Group
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et al.)

Conclusions

- For Cyg OB2 12, $N(1,0) / N(CH^+) \lesssim 0.4$
- Constrains conditions where CH^+ formed
  - – not at low T & high f
  - – not in “normal” diffuse gas?
- Constrains models
  - – “rules out” superthermal H_2
  - – consistent with shocks
  - – consistent with turbulence

$$\frac{n(1,0)}{n(CH^+)}$$

T \ f	0.4	0.5	0.6	0.7	0.8	0.9	1.0
40	0.33	0.46	0.60	0.74	0.88	1.02	1.17
60	0.30	0.41	0.53	0.65	0.77	0.89	1.02
80	0.27	0.36	0.46	0.56	0.66	0.76	0.87
100	0.24	0.32	0.40	0.49	0.57	0.66	0.75
120	0.21	0.28	0.35	0.43	0.50	0.58	0.65
140	0.19	0.25	0.32	0.38	0.45	0.51	0.58
160	0.17	0.23	0.29	0.34	0.40	0.46	0.52
180	0.16	0.21	0.26	0.31	0.36	0.42	0.47
200	0.14	0.19	0.24	0.29	0.33	0.38	0.43
220	0.13	0.18	0.22	0.26	0.31	0.35	0.39
240	0.12	0.16	0.20	0.24	0.28	0.32	0.36
260	0.12	0.15	0.19	0.23	0.26	0.30	0.34
280	0.11	0.14	0.18	0.21	0.25	0.28	0.32
300	0.10	0.13	0.17	0.20	0.23	0.26	0.30

Future Work

- Cygnus OB2 12 seems best bet
  - complete CH_3^+ data reduction
    - improved limit on N(1,0)?
  - complete CH^+ data reduction
    - improved estimate of $N(CH^+)$
- Search for CH_3^+ in more heavily reddened sightlines
  - $N(CH^+)$ may be even higher?
  - better limit on $N(1,0)/N(CH^+)$