Optical/NIR studies of the ISM

I. Interstellar chemistry
   i. Brief history, astrophysical context

II. Diffuse and translucent molecular clouds
   i. unresolved problems from observations

III. Required modifications
   I. CH^+: Non-Maxwellian velocity distributions, XDRs, PDRs
   II. DIBs: change of ionisation balance
   III. H_3^+: X-ray induced chemistry, ionisation rate

IV. Summary
   Better observations required

1

Molecular Astrophysics

- gas phase chemistry in ISM
- IR emission, Dust, surface chemistry
- Comets, pre-biotic organic molecules
- Star formation, HH objects, outflows

Interstellar molecules

I. Brief History

1922	5780, 5797 stationary features (Heger 1922)
1926	Eddington, molecules cannot survive ISRF
1934	Merrill, several strong DIBs detected
1937-39	CH, CH^+, CN: stationary optical absorption lines
1951	Bates & Spitzer, first models (Kramers & ter Haar 1946)
1963	Radio astronomy, OH, NH_3
1970	H_2 Copernicus satellite, UV absorption lines
1973	Herbst & Klemperer, ion-molecule reactions
1975	X-ogen (HCO^+)
2005	some 125 gas-phase molecules confirmed

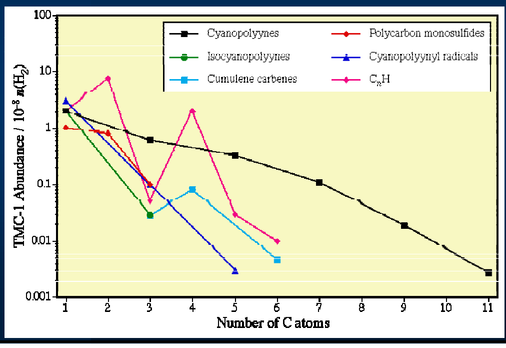
3

Interstellar medium

- **Phase transitions: $H^+ \rightarrow H \rightarrow H_2$**
  - Hot ionised HII: $5\ 10^5$ K, $5\ 10^{-3}$ cm^{-3}
  - Warm HI/HII: 8000 K, 0.3 cm^{-3}
  - Cool atomic: 80 K, 30 cm^{-3}
  - Cold molecular: 10-100 K, 100 - 10^3 cm^{-3}
    - Diffuse interstellar clouds
    - Giant molecular clouds
    - Pressure equilibrium: nT = const

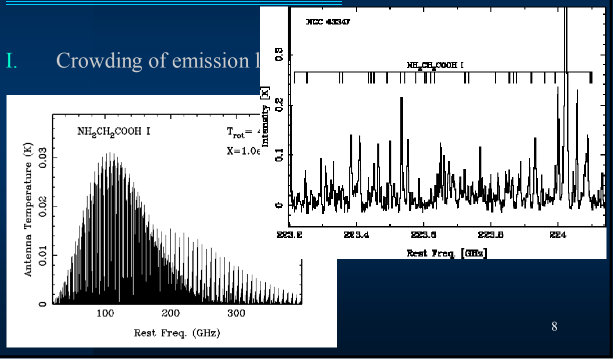
4

Dense molecular clouds



Confusion limit: Glycine

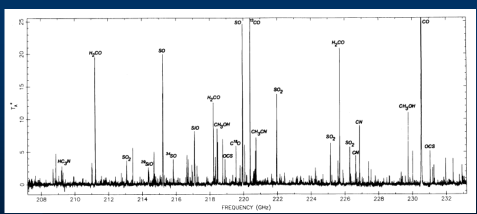
I. Crowding of emission l



Confusion limit: OMC-1

I. Blake et al. 1987, OMC-1

Spectral resolution 0.14 km s^{-1}



Interstellar chemistry

- **Theoretical models**

Interstellar chemistry

- Ion-molecule reactions
  - Ionising source: photons (diffuse clouds), X-rays, cosmic rays (dense clouds)
- Neutral-neutral reactions
- Radiative recombination
  - free electrons required
- Dissociative recombination

- Initiation of gas phase chemistry: H_2 required

Interstellar chemistry

I. $H \rightarrow H_2 \rightarrow H_3^+$

- by radiative association, $H(1s) + H(1s) \rightarrow H_2 + h\nu$
  - Very slow, forbidden in first order for homonuclear molecules
- by grain surface chemistry, $H + H{:}gr \rightarrow H_2 + gr$

$H_2 + CR \rightarrow H_2^+$

$H_2^+ + H_2 \rightarrow H_3^+$

- $H_3^+ + e \rightarrow H_2 + H$
  - **dissociative recombination rate**

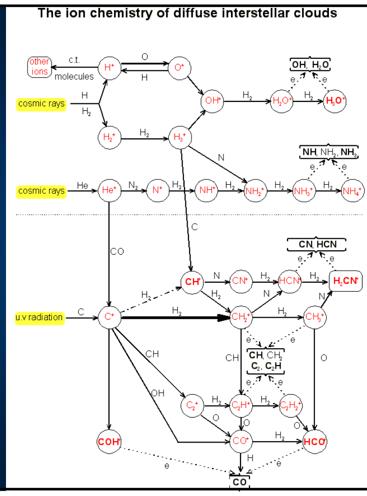
  Fast (Amano 1988, Larsson 2000)

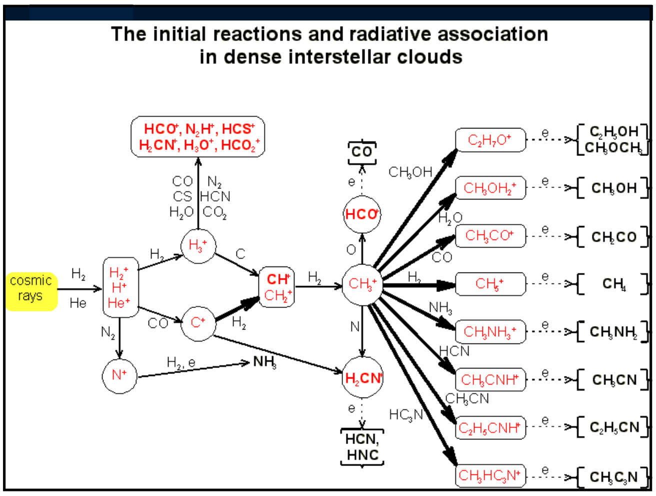
  Slow (Plasil et al. 2003) minority view

Interstellar chemistry

I. Carbon chemistry
   - $C + ISRF\ (IP\ 13.3eV) \rightarrow C^+ + e$
   - $x_e = 10^{-4}$
   - $C^+ + H_2 \rightarrow CH^+ + H \quad \Delta E = 0.4\ eV$
   - $C^+ + H_2 \rightarrow CH_2^+ + h\nu$, radiative association, slow

- Oxygen chemistry
   - $O + H^+ \rightarrow O^+ + H$ charge transfer
   - $O^+ + H_2 \rightarrow OH^+$
- Nitrogen chemistry
   - $N + H_3^+ \rightarrow NH_2^+$ radiative association, slow





Interstellar chemistry

- New Standard Model
   - Bettens 1995, 3785 reactions, 409 species
   - Many reaction rates guessed, often wrong T-extrapolation
   - **$\zeta = 10^{-17}\ s^{-1}$**
- Famous problems remain: DIBs, H_3^+, CH^+
   I. DIBs: carriers not identified
   II. DIBs and H_3^+: major impact on ionisation rates
   III. CH^+: formation scenarios not understood

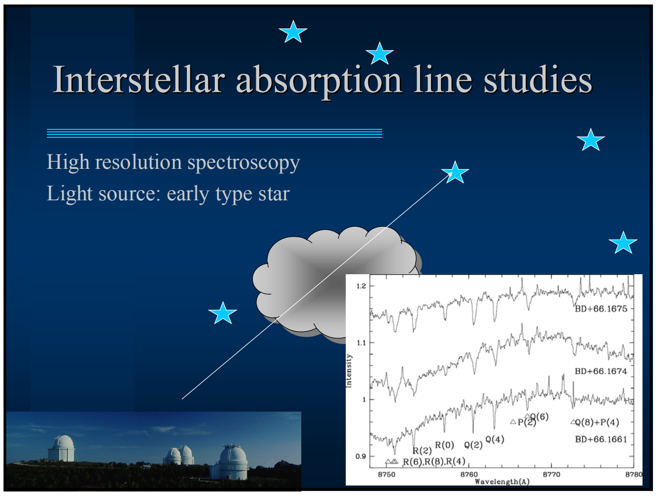
Translucent clouds

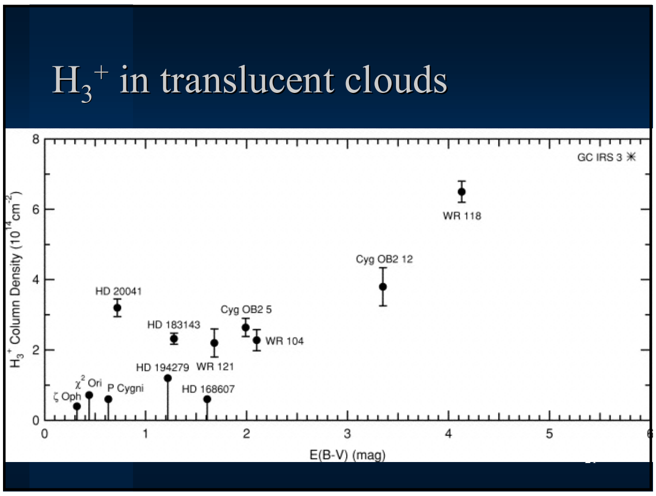
- **Optical/NIR absorption lines**
   - **Interstellar H_3^+**
   - **The DIBs**
   - **Interstellar CH^+**

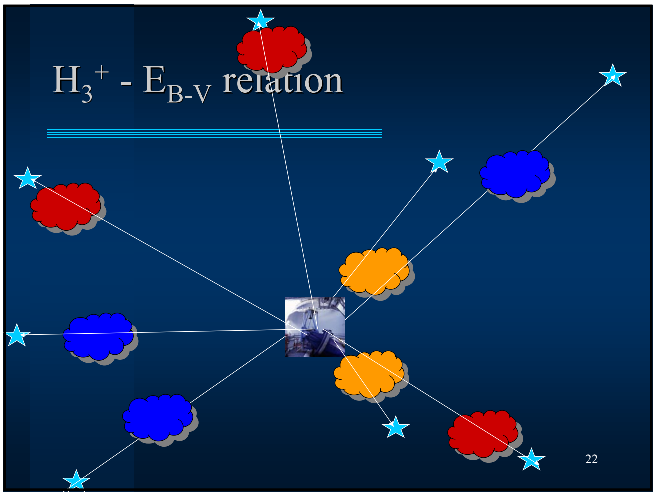
Translucent molecular clouds

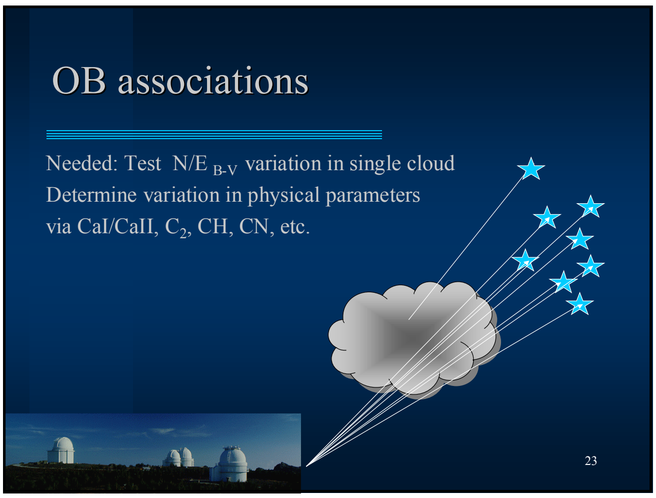
- Diffuse interstellar clouds
   - $A_v < 1$ mag, ionisations from ISRF dominate
- Translucent clouds, edges of giant molecular clouds
   - $A_v = 1 - 5$ mag
      - Background stars still visible
   - $T = 20 - 100$ K
   - $n = 100 - 1000\ cm^{-3}$

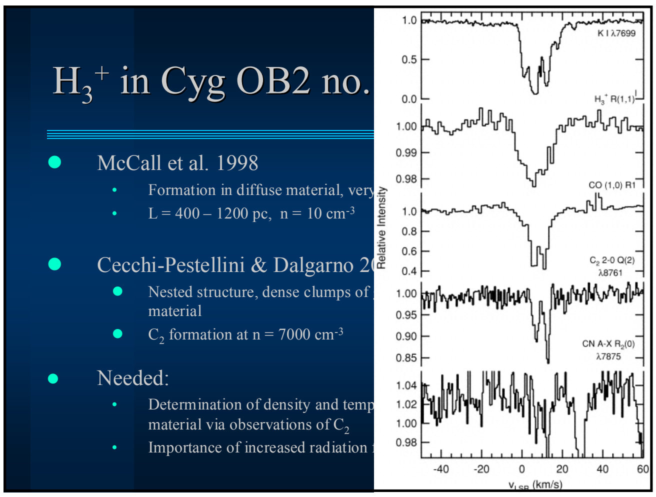

The Horsehead Nebula — Barnard 33
HUBBLESITE.org


Interstellar absorption line studies
High resolution spectroscopy
Light source: early type star
BD+66.1675
BD+66.1674
BD+66.1661
Intensity
Wavelength(A)
8750
8760
8770
8780

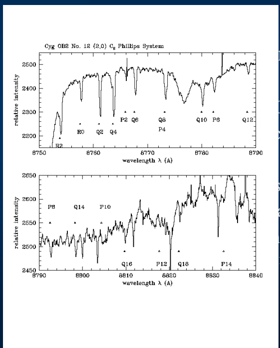

H_3^+ in translucent clouds
H_3^+ Column Density (10^{14} cm^{-2})
E(B-V) (mag)
GC IRS 3
WR 118
Cyg OB2 12
HD 20041
HD 183143
Cyg OB2 5
WR 104
HD 194279
WR 121
HD 168607
χ^2 Ori
P Cygni
ζ Oph

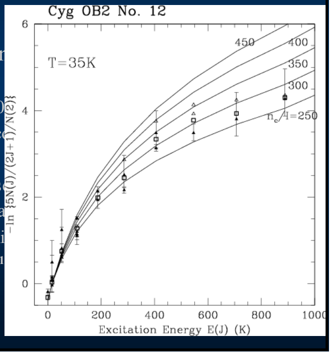

H_3^+ - E_{B-V} relation
22


OB associations
Needed: Test N/E $_{B-V}$ variation in single cloud
Determine variation in physical parameters
via CaI/CaII, C_2, CH, CN, etc.
23


H_3^+ in Cyg OB2 no.
McCall et al. 1998
Formation in diffuse material, very
L = 400 – 1200 pc, n = 10 cm^{-3}
Cecchi-Pestellini & Dalgarno 2
Nested structure, dense clumps of
material
C_2 formation at n = 7000 cm^{-3}
Needed:
Determination of density and temp
material via observations of C_2
Importance of increased radiation
K I λ7699
H_3^+ R(1,1)
CO (1,0) R1
C_2 2-0 Q(2) λ8761
CN A-X R_2(0) λ7875
Relative Intensity
v_{LSR} (km/s)

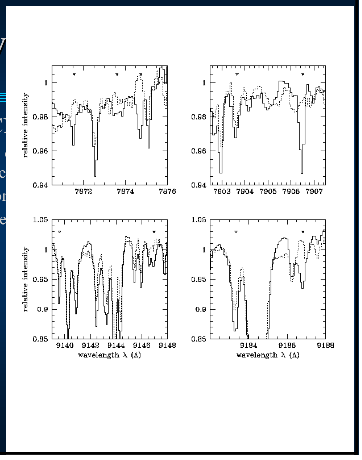
C_2 towards Cyg OB2 no. 12





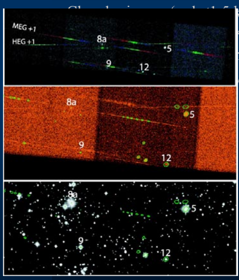
CN towards Cy

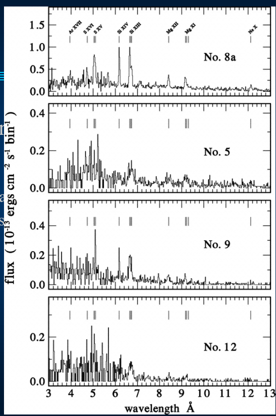
- Large abundances of C
  - CN formation requires
    Gredel Pineau des Fore
  - Velocities of absorption
  - Formation of H_3^+ in de



Cyg OB2

- Modelling of radiation field i





X-ray induced chemistry

- Cool molecular clouds subjected to X-rays
  Gredel, Lepp & Dalgarno 1987, Gredel, Yan & Black 2001
- $M + xr \rightarrow M^{2+} + 2e$
  - $C^{2+} + H_2 \rightarrow CH^+ + H^+$
  - $S^{2+} + H_2 \rightarrow SH^+ + H^+$
  - O^{2+} rapid charge transfer to H, H_2, reduced to O^+
  - $CO + h\nu \rightarrow C^{2+} + O + e_f + e_a$
  - $\rightarrow O^{2+} + C + e_f + e_a$
- Energy deposition by fast secondary electrons
  - Gredel & Dalgarno 1995
  - Coulomb losses to thermal electrons
  - Ionisation and excitation of H and H_2
  - He, n→ 2, 3 singlet and triplet S and P states and to 4^1P

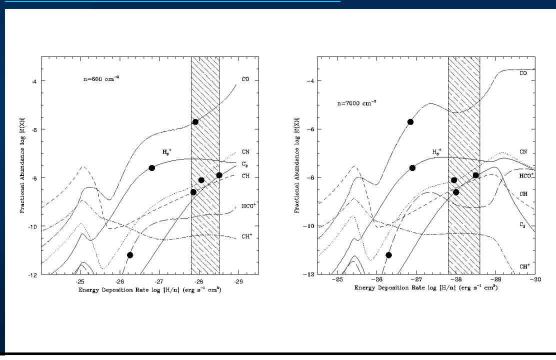
28

CR & X-ray induced chemistry

- Radiation field in dense molecular clouds
  i. Energetic, secondary electrons from CR or X-ray ionisation
  ii. $H_2 + e \rightarrow H_2^*$
  iii. $H_2 \rightarrow H_2(vJ)$ + UV-photons (Lyman and Werner bands)
  iv. $H_2(vJ) \rightarrow H_2$ + NIR-photons (E2 cascade)
- Increased photoionisation and photodissociation rates
  - Explains C/CO ratio in dense clouds
- **X-rays: chemistry modified by**
  - Double charged ions drive reactions
  - Induced, diffuse UV radiation field increase photodissociation and photoionisation rates

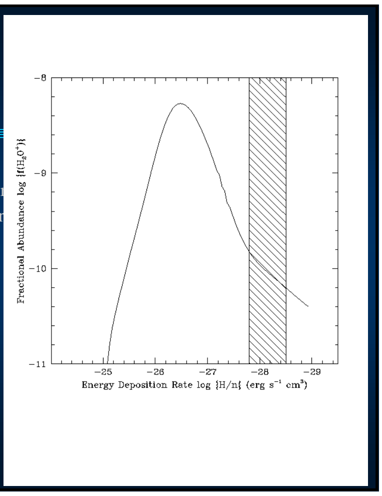
29

Cyg OB2 no. 12



Cyg OB2 no.

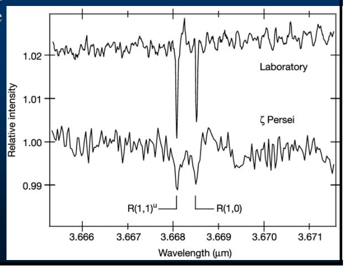
- Model prediction:
  - Observable amou
  - S/N > 1000 spectr



H_3^+ in the diffuse ISM

- McCall et al. 2003
  - Large abundance in diffuse cloud towards ζ Per
  - dense molecular clouds: $\zeta = 3\ 10^{-17}\ s^{-1}$
  - Cosmic ray ionisation rate
  - $\zeta = 1.2\ 10^{-15}\ s^{-1}$

I. general solution
ζ: $10^{-17}\ s^{-1}$ → $10^{-15}\ s^{-1}$



The ironic twists in H_3^+

I. Lepp et al. 1988, large molecules
- Chemical models including photoelectric heating of LM: large, observable abundance of H_3^+
  Wrong. slow recombination rate used
- Did not stimulate observations to detect H_3^+

II. New laboratory measurements: H_3^+ + e very fast
- Models: H_3^+ abundance too low to be detected
- Stimulated huge observational efforts to detect H_3^+

III. 2003: large abundance of H_3^+ detected in diffuse ISM
Ionisation rate must be increased

Optical/NIR absorption line studies

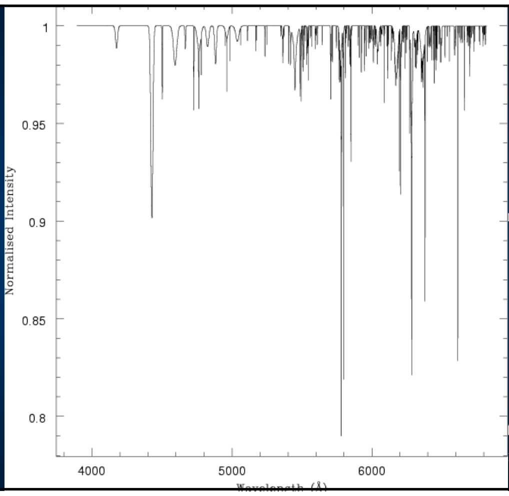
C_2 homonuclear molecule
- thermal population among X v=0 J=0,2,4 → T_{kin}
- A-X Philips system and intercombination transitions → n

CN violet – red system
- Doppler b values, n, n_e

CaI/CaII
- electron densities

CH
- hydrogen column density

H_3^+
- ionisation rates



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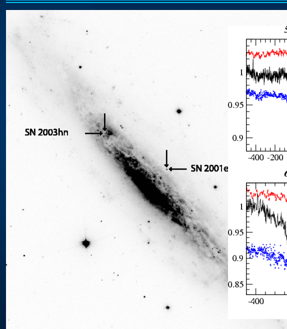
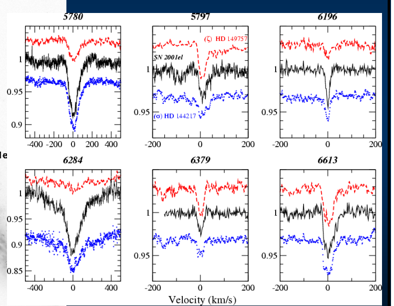
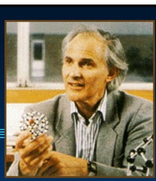
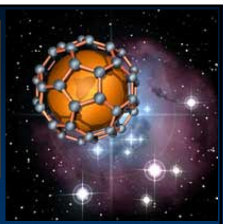
The diffuse interstellar bands





DIB carriers





- Carriers of DIBs
  - Sir Harold Kroto Sussex, 1996 Nobel Laureate Chemistry C_{60}
- Fundamental role in ionisation balance
  - Liszt 2003 PAH grain neutralisations
    - Heating balance: radiative and dielectronic recombination of charged ions
    - $PAH^- + H^+ \rightarrow PAH + H$ rapid destruction of protons

Ionisation rate must be increased

37

The CH^+ problem

- $N_{obs}/N_{model} = 1000$
  - $C^+ + H_2 \rightarrow CH^+ + H$ $\Delta E = 0.4$ eV
- Thermal formation scenarios
  - Elitzur & Watson 1978, 1980: J-type shocks
  - Pineau des Forets et al. 1986: C-type shocks
  - Dissipation of interstellar turbulence, boundary layers
- Predictions & earlier observations
  - CH – CH^+ large velocity difference expected
  - $N(CH^+)$ not correlated with E_{B-V}

38

The CH^+ problem

L20 LAMBERT, SHEFFER, AND CRANE Vol. 359

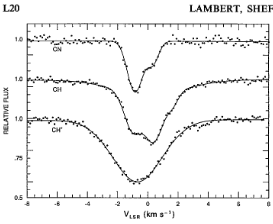


FIG. 1.—Profiles of the CN 3874 Å, CH 4300 Å, and CH^+ 4232 Å lines in the spectrum of ζ Oph. The CN and CH profiles have been shifted so that the stronger of the two narrow components is at $V_{LSR} = -0.79$ km s^{-1}, the velocity of the stronger CO component. The solid lines show the least-squares–fitted profiles.

strength $\frac{2}{3}$ and $\frac{1}{3}$. The velocity splitting between the two main

CN line. The small difference between the velocities of the CN and CO main components may not be real. Since our reference spectrum from a hollow cathode lamp probably does not illuminate the spectrometer in the same way as a star, a small velocity error is possible. In addition, the difference of 0.3 km s^{-1} is equivalent to an error in the CN line's adopted wavelength (Black and van Dishoeck 1988) of only 3.9 mÅ.

Langer, Glassgold, and Wilson (1987) observed the CO $J = 1$–0 line with a 1'.7 beam and deconvolved the line into three main components and one weak component. When we fitted the CN line to a three-component model, an adequate fit is obtained, but the required line widths are larger than the 0.50–0.58 km s^{-1} widths obtained by Langer *et al.* The additional components found by Langer *et al.* are probably artifacts of their larger beam size; Le Bourlot *et al.* clearly show that the velocity of their weak component varies on scales smaller than Langer *et al.*'s beam.

b) CH^+ Profile

The CH^+ at 4232 Å is very well fitted by a single Gaussian profile with a FWHM of 3.49 ± 0.09 km s^{-1}. The equivalent width from our observations is $W_\lambda = 23.1 \pm 0.3$ mÅ. The measured velocity of the CH^+ line is $V_{LSR} = -0.9 \pm 0.5$ km s^{-1} where the Moon provided the reference spectrum. We adopt $V_{LSR} = -0.7$ km s^{-1} (Lambert and Danks 1986). The rest

The CH^+ probl

- **ζ Oph is an excep**
  - Velocity difference
  - $N(CH^+)$ not correla
  - Allen 1994, Falgar

line indicates an equivalent width of 20 mÅ, and the dashed line indicates 43 mÅ. A small additional error of about 0.1 dex is introduced by selecting a *b* value which is lower than the true value, since the curves nearly overlap. Choosing a *b* value which is too large is a more serious problem. As the figure shows, it is possible to have column density errors which are greater than 0.5 dex.

We plotted the calculated CH^+ values, along with our observations in Figure 7. The figure shows that, when $E(B-V)$ is extended past +1.0, it now does not appear that CH^+ continues to increase with reddening. This is of particular interest in that it supports the shock model, or any other model in which CH^+ is formed in thin layers of the ISM instead of throughout the material. Increasing column density implies that we are looking through higher and higher optical depths of material as $E(B-V)$ increases. Since shock-formed CH^+ is only expected to be produced in relatively thin layers of the ISM, increasing optical depth will not substantially increase

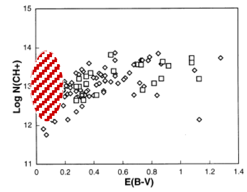
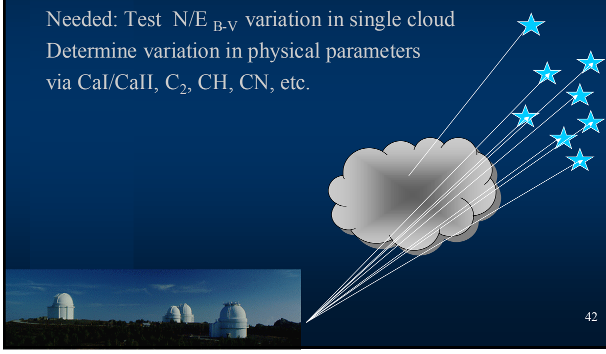


FIG. 7.—CH^+ column densities versus reddening. The diamonds indicate the observations listed in Table 7. The squares are the new observations described in this paper.

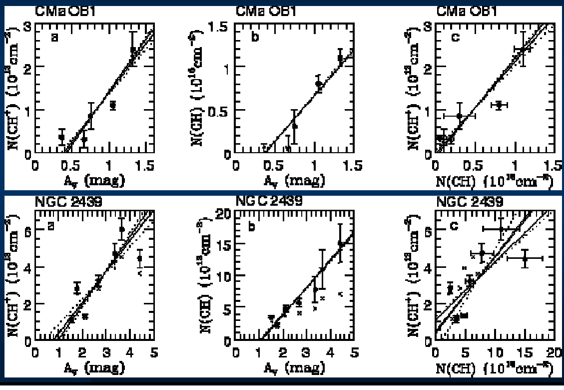
OB associations

Needed: Test N/E $_{B-V}$ variation in single cloud
Determine variation in physical parameters
via CaI/CaII, C_2, CH, CN, etc.



42

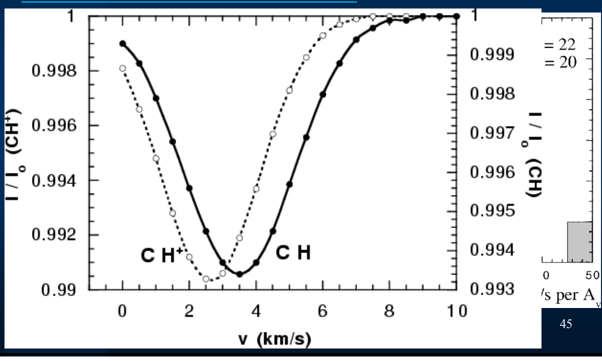
The CH⁺ problem



The CH⁺ problem

- $N(CH^+) \sim E_{B-V}$
  - Tight correlation in single translucent clouds
  - Correlation is absent if sample contains too many different lines of sight
  - Pleiades, Cep OB4: correlation absent
- Radial velocities agree within errors
  - Earlier results with $v(CH) - v(CH^+) > 4$ km s^{-1} cannot be reproduced: upper limit to shock velocities
- C_2 observations → n, T
  - CH^+ formation sites in cool gas

Interstellar CH⁺



Summary

I. CH^+ formation: mystery remains
   I. Single shocks don't work
      I. Firm statement after systematic studies in single translucent molecular clouds
   - Dissipation of turbulence
      I. CH^+ formation in cool gas
      II. Non-Maxwellian chemistry from super-thermal C^+ or H_2
      III. Multiple, criss-crossing shocks at low velocities, no strong heating
   I. Fast formation in high-ionisation zones
      I. Not the general formation scenario

Summary

I. DIBs
   I. Huge progress in recent years
   II. PAHs, PAH cations
   III. Needed
      I. Systematic studies of single clouds, determination of physical parameters using diatomics and ions
      II. Accurate laboratory wavelengths required
      III. He clusters, very low matrix shifts and broadening
   IV. Dramatic effect on ionisation equilibrium

Summary

I. H_3^+
   I. Very large abundances in diffuse and dense clouds
   II. Chemistry well understood
   III. Significant increase in ionisation rate required