Probing The Chemistry And Dynamics Of Hot Molecular Cores Using Cyanopolyynic Transitions

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Overview

- Background
- Non-LTE hyperfine radiative transfer analysis
- Chapman's 2009 model
- COLHYPOD (a scant review!)
- Future Aims

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   - Molecular Line Emission
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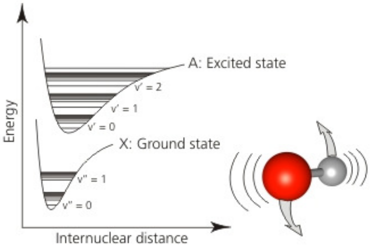
Observing Molecular Cloud Cores

- Stars form inside cold ($\approx$10K) dense (10^4-10^6cm^{-3}) dusty "cores" in molecular clouds
- These cores are highly obscured (optically opaque) so need to observe in mm or sub-mm regimes HCN J=1$\rightarrow$0 @ 0.338mm HCO^+ J=1$\rightarrow$0 @ 0.342mm
- Continuum observations detect the dust emission
- Line observations (from gas phase molecules or ions) trace the gas and its dynamics

Molecular Spectroscopy

Molecular spectra can be due to a combination of:

- Molecular rotations – collective motions of atomic nuclei within the molecule – microwave + mm-wave regions
- Molecular vibrations – relative motions of the atomic nuclei – IR spectroscopy
- Electronic excitations – transitions amongst potential energy surfaces – visible and UV spectroscopy



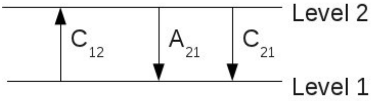
Molecular shape is unique – creates a unique energy structure – leading to unique transitions that help identify the emitting molecule

Molecular Line Emission

In star-forming regions:

- Physical conditions – excitation conditions depend on T_{kin}, n_{H_2} and the ambient radiation field
  - Molecular Clouds: T_{kin} $\sim$10K $\rightarrow$ excites the lowest rotational transitions
  - From line intensities: T_{ex} and N_{col}
- Kinematics – linewidths and morphology: turbulent and systemic motions of the gas
- Stage of the evolution – Time-dependent chemistry and spatial distribution of some species (e.g. NH_3 (late-type) and CCS (early-type molecule))

Two-Level Atom 1

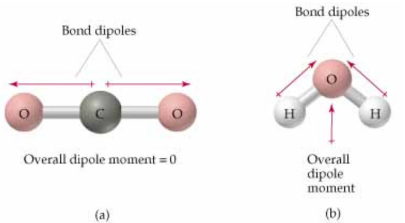


$$(A_{21} + C_{21}n)\, N_2 = C_{12} n N_1$$

$$\frac{N_2}{N_1+N_2} = \frac{C_{12}/C_{21}}{1+\frac{A_{21}}{C_{21}n}+C_{12}/C_{21}} = \frac{\frac{g_2}{g_1}e^{-\left[\frac{E_2-E_1}{kT}\right]}}{1+\frac{n_{cr}}{n}+\frac{g_2}{g_1}e^{-\left[\frac{E_2-E_1}{kT}\right]}}$$

where $n_{cr} = A_{21}/C_{21}$ is the critical density. When $n \gg n_{cr}$, the level population is given by the Boltzmann distribution. If $n \ll n_{cr}$, upper-level population smaller than expected for the Boltzmann distribution. Such a low-density gas emits only weakly.

Two-Level Atom 2



Nitrogen bearing molecules have large dipole moments (μ):-
HCN(μ=2.985D) - N_2H^+(μ=3.37D) - NH_3(μ=1.47D)
(1D = 10^{-18}esu-cm)
The Einstein A value – proportional to μ^2 – large for N-bearing molecules $\Rightarrow$ the critical density of the J=1$\rightarrow$0 transition for each of these species can be as high as 10^6cm^{-3} – trace the advanced stages of core contraction.
Also, A $\propto$ $(J+1)^3$ $\Rightarrow$ n_{crit} $\uparrow$ for higher transitions.

Hyperfine Structure

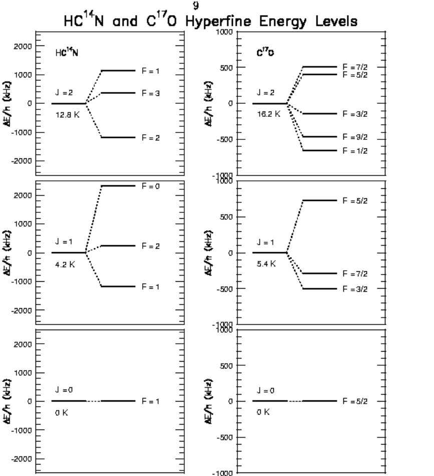


Fig. 7. The hyperfine energy level structure of HCN and $C^{17}O$ for J = 0, 1, and 2. The vertical axisistheshift in energy($\Delta E = E_Q + E_M$) in kHz. Note the vertical scale is different for HCN and $C^{17}O$.

Nonspherical positive nuclear charge of ^{14}N (I_N=1) ⇒ electric nuclear quadrupole moment

Interacts with the negative electron field giving rise to sizeable hyperfine structure

Additional contribution - nuclear spin rotation interaction = $\vec{B}$-field generated by rotating charged particles + nuclear spin of the ^{14}N isotope.

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Accounting for Hyperfine Structure

Condition for Local Thermodynamic Equilibrium:

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} \exp\left(\frac{E_{ul}}{kT_{kin}}\right)$$

When LTE conditions do not hold within moderate density regimes and considering the typical abundances of nitrogen-bearing species in the gas phase, the total opacity of observed rotational transitions for these species should be derived considering their hyperfine structure.

Errors in derived opacities and column densities can be as large as 100%, F. Daniel et al. 2006.

Cyano-species and their hyperfine structures I

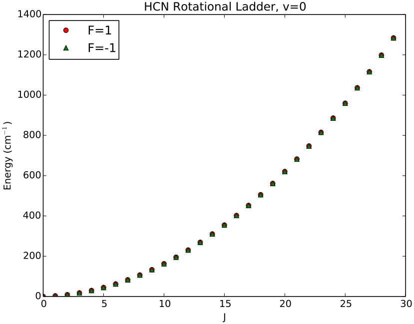
Observing cyanopolyynic transitions has the following advantages:

- Several transitions are observable simultaneously in a given waveband
- Large dipole moment requires large critical densities for excitation $\rightarrow$ trace highly opaque regions
- Can be used to assign a particular stage of evolution to an observed source of emission

Cyano-species and their hyperfine structures II

HCN hyperfine energy structure via Ahrens et al. (2002), Eq. (5):

$$E(J,F) = E_{\mathrm{rot}}(J) + E_{\mathrm{quad}}(J,F) + E_{\mathrm{spin\text{-}rot}}(J,F)$$
$$= \mathbf{B}J(J+1) - \mathbf{D}[J(J+1)]^2 + \mathbf{H}[J(J+1)]^3$$
$$- \mathbf{eQ}\cdot(\mathbf{q}_0 + \mathbf{q}_\mathrm{J})\left\{\frac{3}{4}C(C+1) - J(J+1)I_\mathrm{N}(I_\mathrm{N}+1)\right\}$$
$$\cdot [2I_\mathrm{N}(2I_\mathrm{N}-1)(2J-1)(2J+3)]^{-1}$$
$$+ [\mathbf{C}_\mathrm{N} + \mathbf{C}_\mathrm{NJ}J(J+1)]C/2, \qquad (5)$$



Cyano-species and their hyperfine structures III

HCN hyperfine energy structure via Ahrens et al. (2002), Eq. (5):

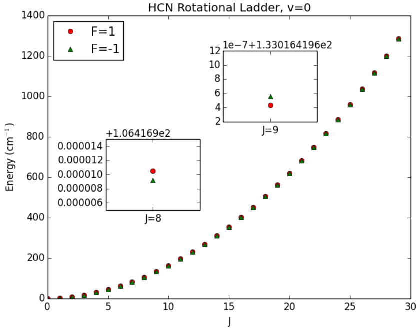
$$E(J,F) = E_{\rm rot}(J) + E_{\rm quad}(J,F) + E_{\rm spin\text{-}rot}(J,F)$$

$$= \mathbf{B}J(J+1) - \mathbf{D}[J(J+1)]^2 + \mathbf{H}[J(J+1)]^3$$

$$- \mathbf{eQ}\cdot(\mathbf{q}_0 + \mathbf{q}_J)\left\{\frac{3}{4}C(C+1) - J(J+1)I_N(I_N+1)\right\}$$

$$\cdot [2I_N(2I_N-1)(2J-1)(2J+3)]^{-1}$$

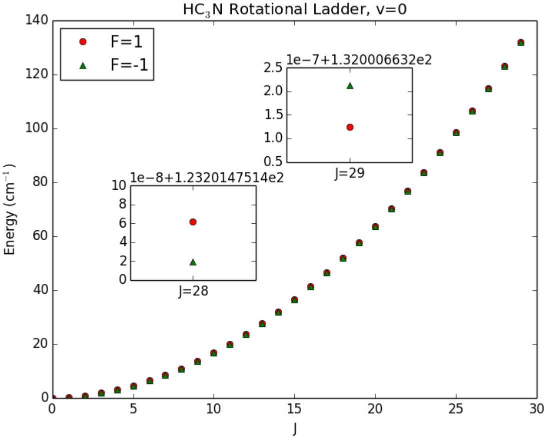
$$+ [\mathbf{C}_N + \mathbf{C}_{NJ}J(J+1)]C/2, \qquad (5)$$



Cyano-species and their hyperfine structures IV

HC_3N hyperfine energy structure:

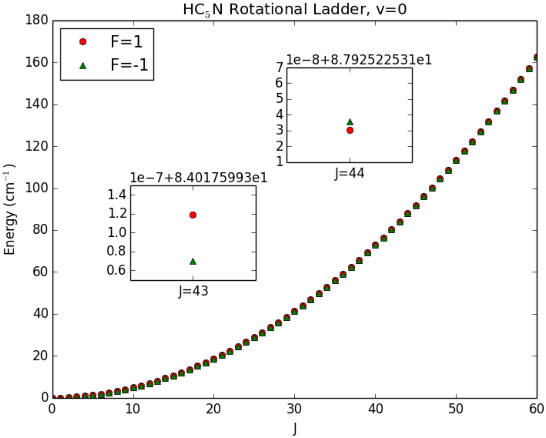
Adopted B, D, eQq and C_N from DeLeon & Muenter 1985.



Cyano-species and their hyperfine structures V

HC_5N hyperfine energy structure:

Adopted B, D, eQq from Gardner & Winnewisser 1978 and adapted C_N from HCN value using scaling factor $B_{0,HCN}/B_{0,HC_5N}$.



CH_3CN Hyperfine Structure I

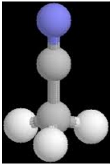
Prolate symmetric rotor species - no inversion lines available on account of structure.

CH_3CN quadrupolar hyperfine energy levels determined using Cazzoli & Puzzarini 2006

Lamb-Dip analysis Centrifugal distortion term for eQq an order of magnitude too large – Müller et al. 2009

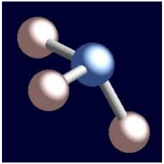
Additional accuracy in rotational level determination using octic and decic terms.

CH_3CN



Prolate symmetric top, does not undergo inversion

NH_3



Oblate symmetric top, does undergo inversion

CH_3CN Hyperfine Structure II

For moderate J, quadrupolar hyperfine transition frequencies are similar for different values of K.

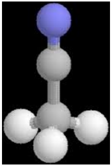
Presented a coding issue - dealt with by treating different (J,K), (J,K'), etc. in similar manner to hyperfine lines.

$J_K = 12_0 \rightarrow 11_0$ - 220.74545GHz

$J_K = 12_1 \rightarrow 11_1$ - 220.74120GHz

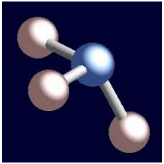
$J_K = 12_2 \rightarrow 11_2$ - 220.72843GHz

CH_3CN



Prolate symmetric top, does not undergo inversion

NH_3



Oblate symmetric top, does undergo inversion

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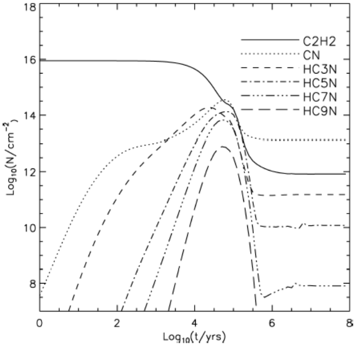
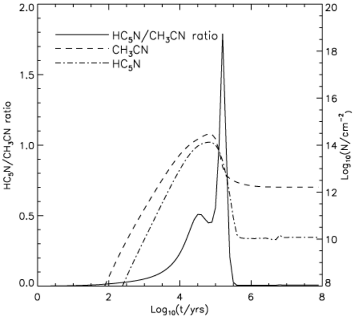
Chapman's 2009 Model I



Strong time-dependence of HC_5N/CH_3CN ratio and hike in cyanopolyynic abundances upon depletion of C_2H_2 used as chemical clock.

Chapman's 2009 Model II



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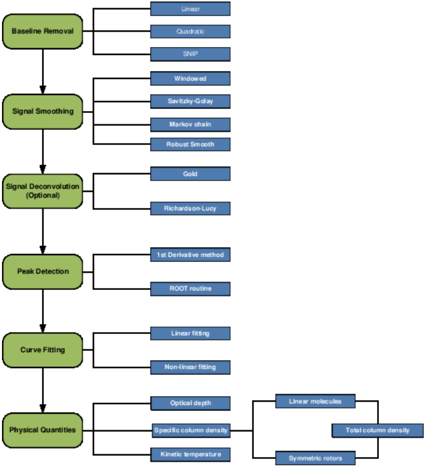
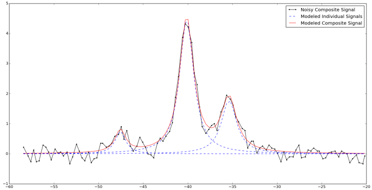


COLumn density determination using HYPerfine structure components to estimate Optical Depth



Pirogov 1999 - IRAS 03035+5819

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Future Aims

- Will complete a parameter sweep of hot core conditions to match closely observations of individual sources
- Aim to produce a plot of derived abundances for HC_5N and CH_3CN, in particular, similar to Chapman's plots - use to estimate core age
- Complete beta testing of COLHYPOD in the Autumn - derive unique T_{ex} for non-overlapping hyperfine components

Thanks for your attention!

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