# *Modeling (Massive) Star Forming Regions*

**Steven Doty**

**Denison University**

*Collaborators: E. F. van Dishoeck, A. Boonman, F. F. S. van der Tak, P. Staeuber, E. A. Bergin, A. O. Benz, and many others*

# Outline

Background & Drivers *(Scientifically, Operationally)*

Modeling Approach

Dust / gas microphysics

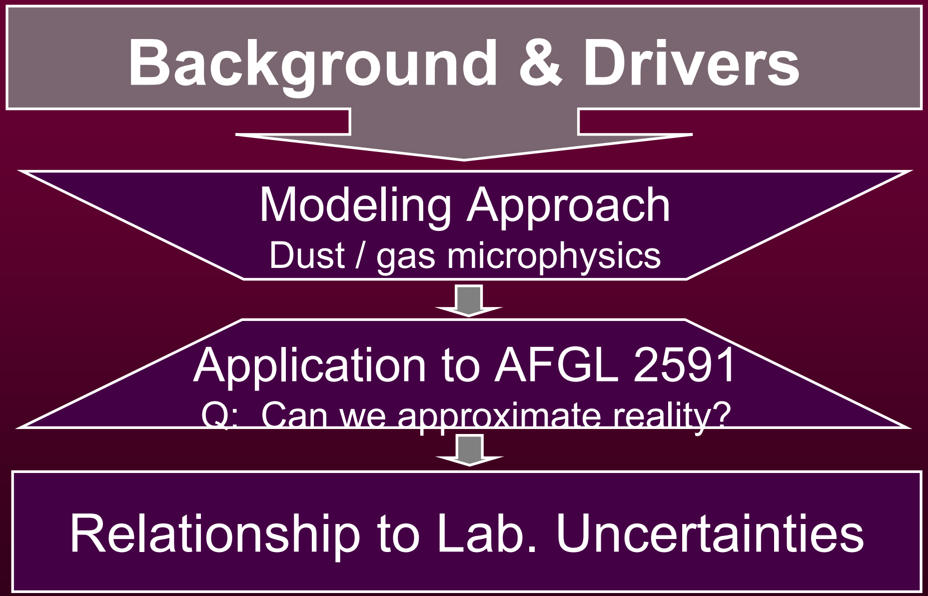
Application to AFGL 2591

Q: What can we infer?

Relationship to Lab. Uncertainties

# *Background & Drivers*

Q: What are the questions at hand, and the motivations for studying them?



# *Drivers*

## *Current Science Question*

Can we understand the structure, origin, and evolution of star-forming regions?

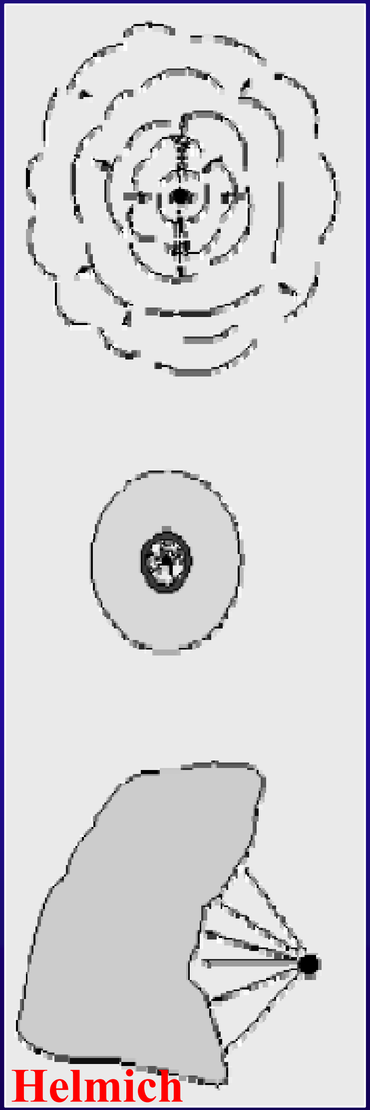
## *Future Unknown Questions*

Can we develop a sufficient straw-man model for the vast upcoming data resources to poke at?

What input (molecular data) uncertainties can be tolerated in the modeling?

# *Star Formation: A Current View*

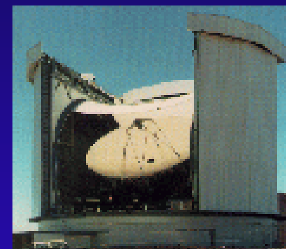
- Pre star-forming cores:
  simple species, T≈10-20 K, n≈$10^4$ cm$^{-3}$,
  t ≈$10^5$-$10^6$ yr (origin?; quasi-static / transient?)
- Collapse phase:
  molecules condensed on grains, T≈10 K,
  n≈$10^5$-$10^8$ cm$^{-3}$, t ≈$10^4$ yr (triggering?)
- YSO phase:
  Evaporation, T≈10 - >200 K, n≈$10^5$-$10^8$ cm$^{-3}$,
  t ≈$10^5$ yr (grain chemistry?; evolution?)
- Outflows:
  Shocks, high-T chemistry, destruction of grain cores: T≈200-2000 K, n≈$10^5$-$10^8$ cm$^{-3}$,t ≈$10^5$ yr



**Helmich 1996**

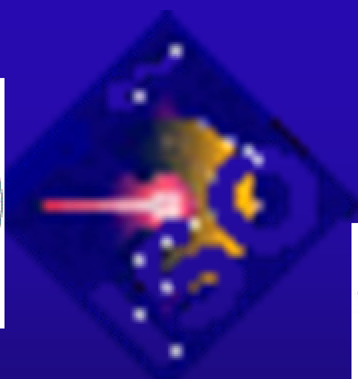
# The (Good!) Problem: Data

Gnd



Air

Spc






~Now

# *Modeling Challenge*

## *Good news*

HUGE amounts of high precision data, allows testing of models

## *Bad news*

HUGE amounts of high precision data, allows testing of models

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Modelers choice: consider 1% of data/sources, or be forced to consider coupled problems

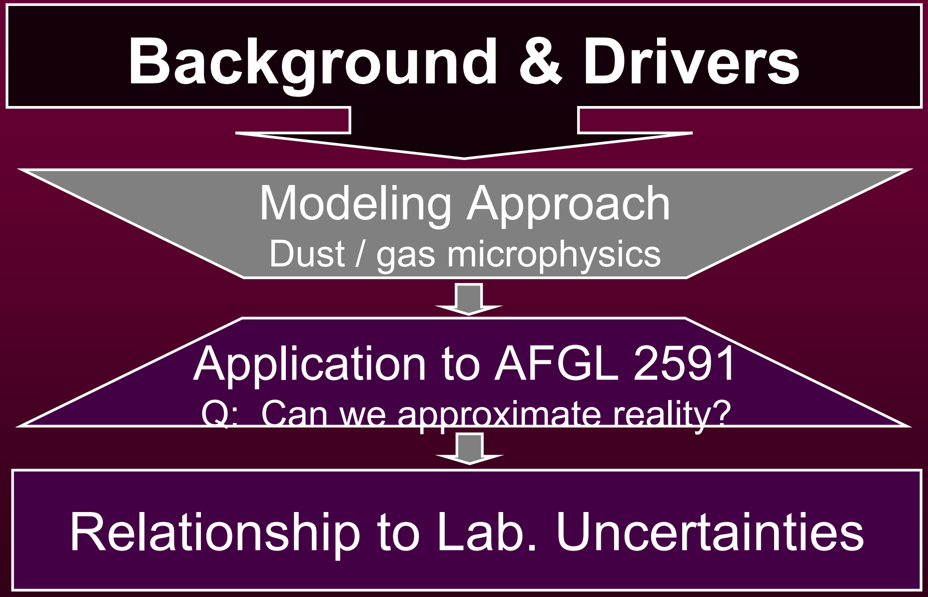
Combined effects of physical, thermal, chemical structure & rad. x-fer ⇒ Comprehensive Modeling

# *Motivation: Summary*

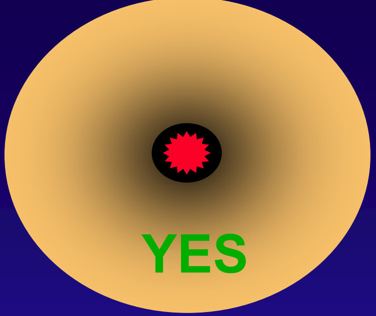
- Goal:  Understand structures of s.f.r.s
- Observational data is pushing analysis
- Models necessary to help interpret the observations
- Basic microphysical understanding necc. before attacking next level of complexity

# *Modeling Approach*

Q: What microphysics and modeling path do we apply to the problem?




# *Modeling Approach*




Treat simplest problem first *(microphysics)*

– spherical with density gradient

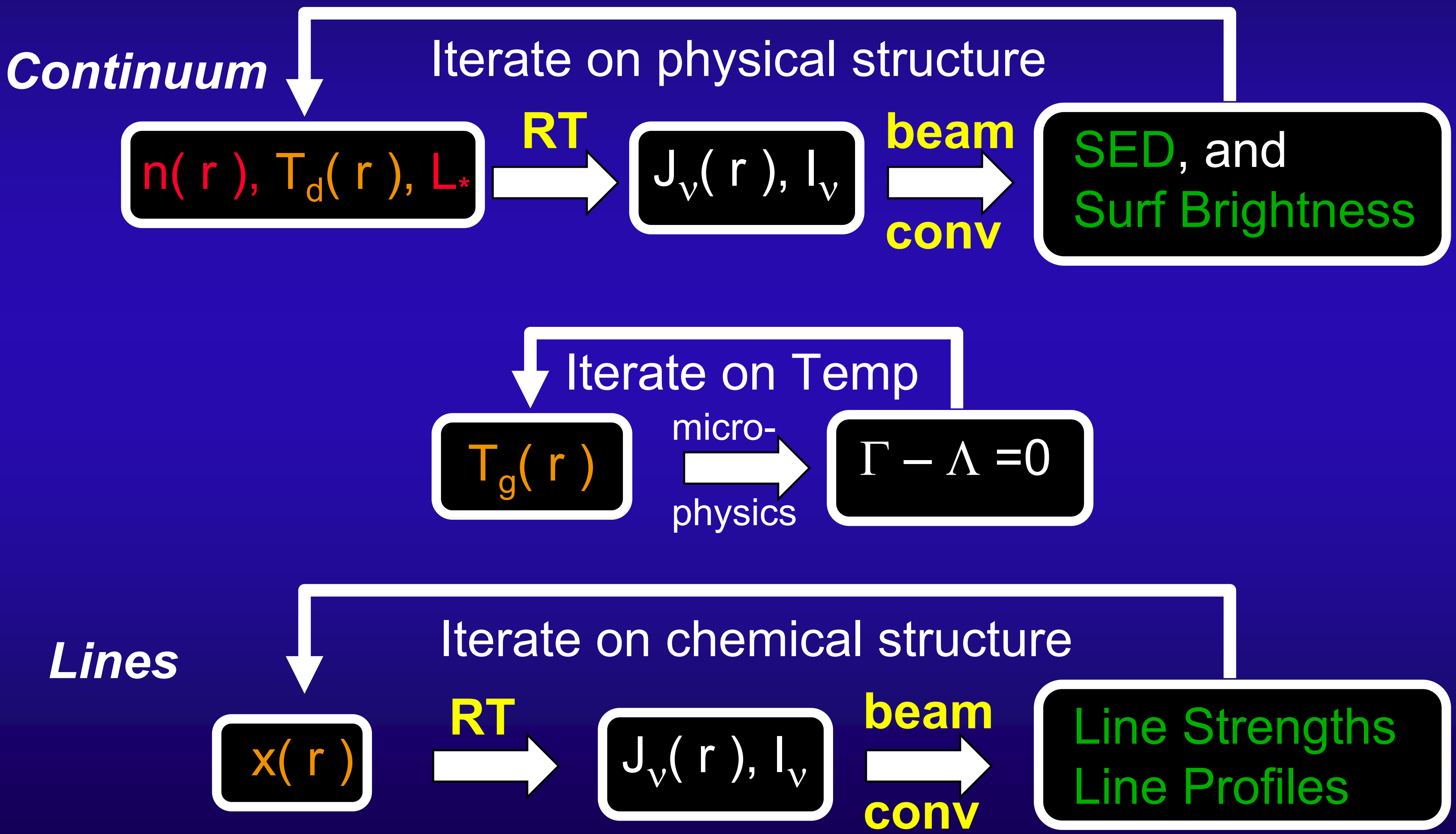
The model includes:

– thermal balance
– detailed chemistry & chemical parameterization
– self-consistent radiative transfer for both lines and continuum

Approach:

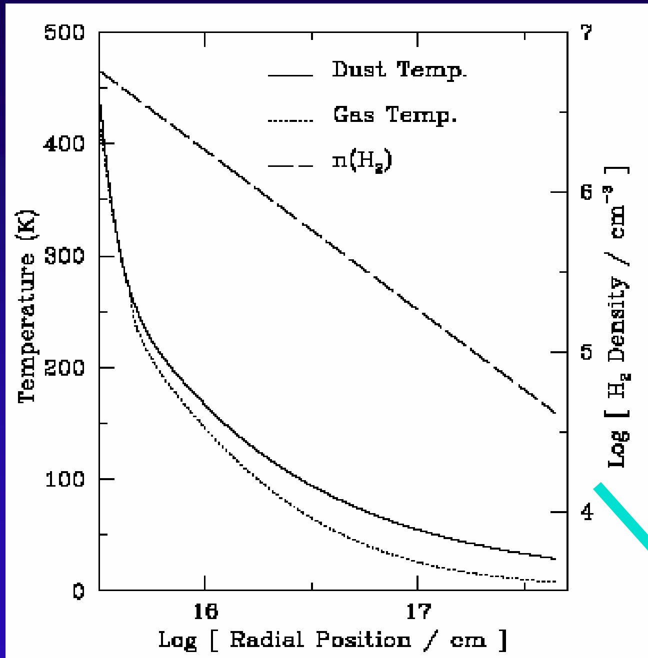
Use multiple observations with detailed model (simulated obs.) to constrain source properties

# *Schematic Diagram of Model*

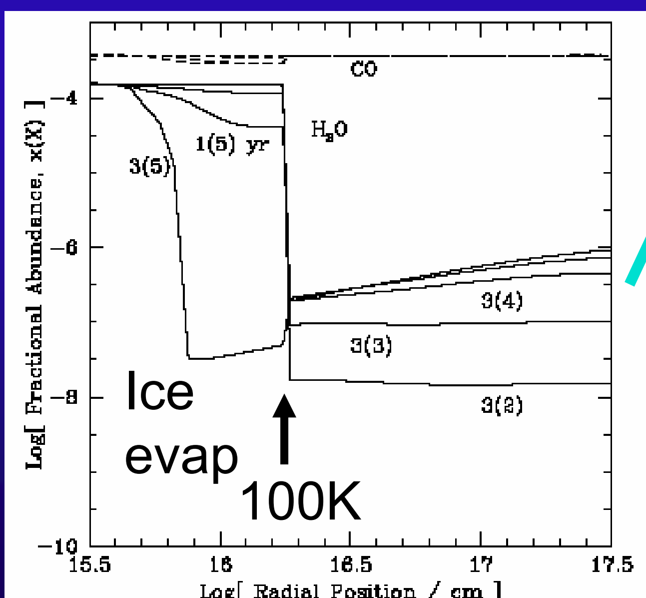


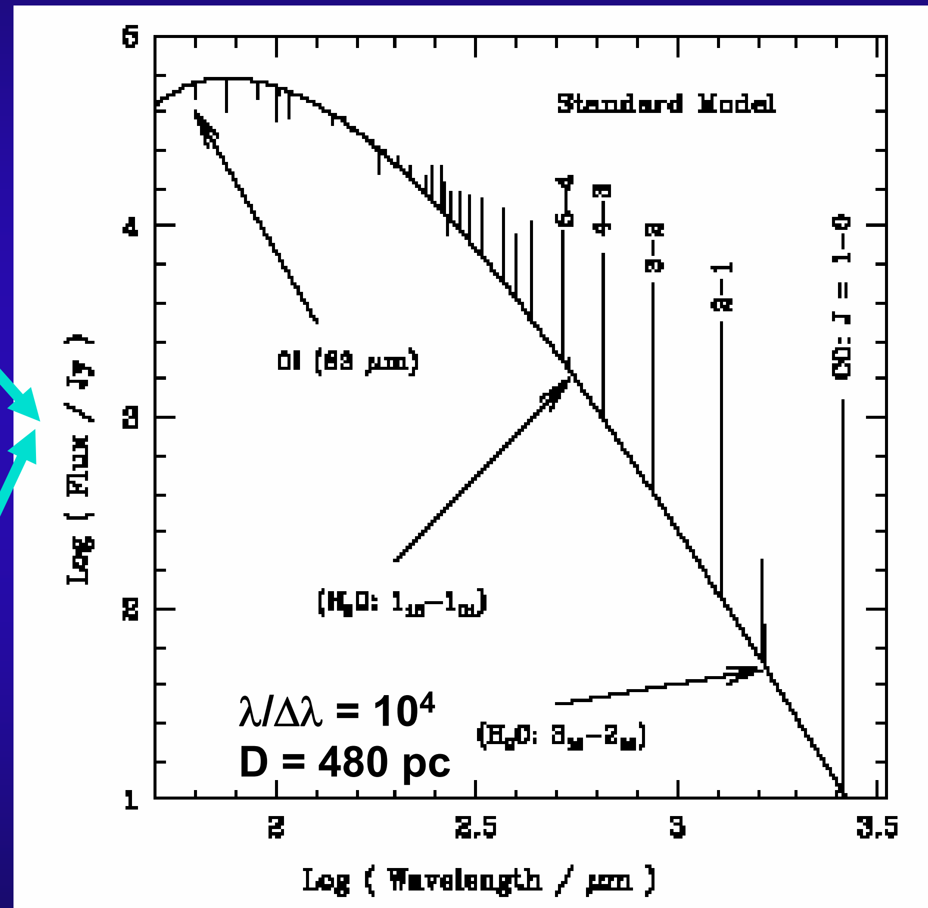
# *Model Outputs: Internal & External*

Physical-thermal structure




Chemical structure

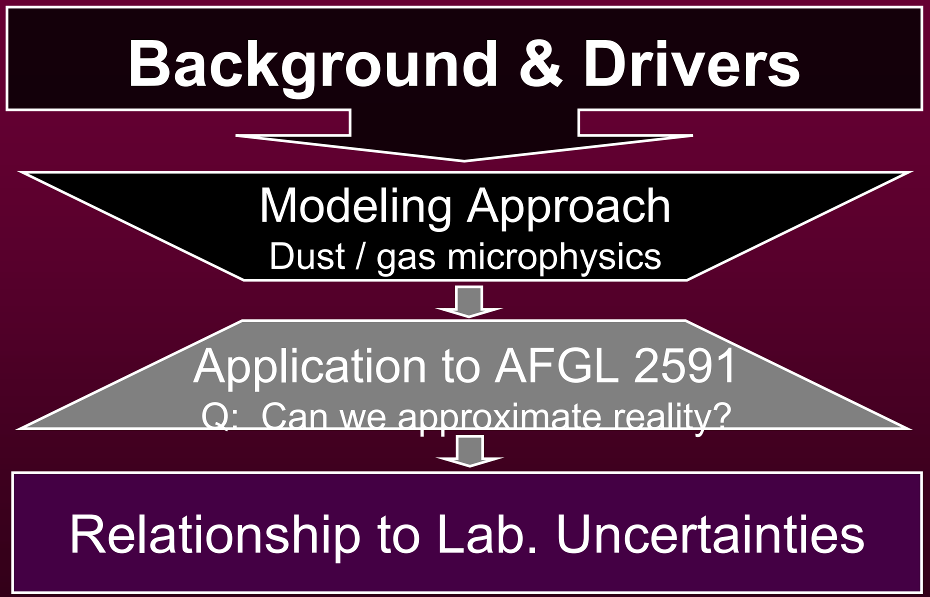


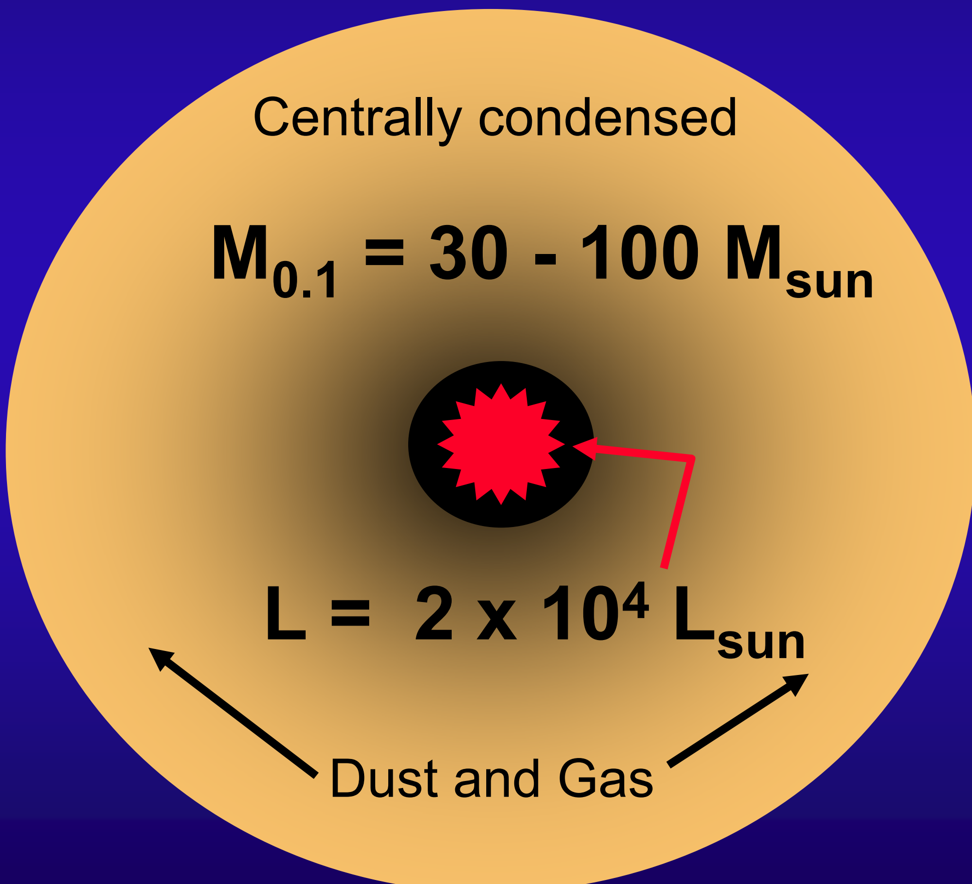

Emergent Spectrum

# *Application to AFGL 2591*

Q: Can we approximate reality?



# Application to AFGL 2591: A Good Testbed




## *Source Properties*

- Massive star-forming region
- Volume not shock dominated
- Well-observed

  ISO-LWS
  ISO-SWS
  SWAS
  JCMT

n( r ) constrained by obs. [van der Tak et al.]

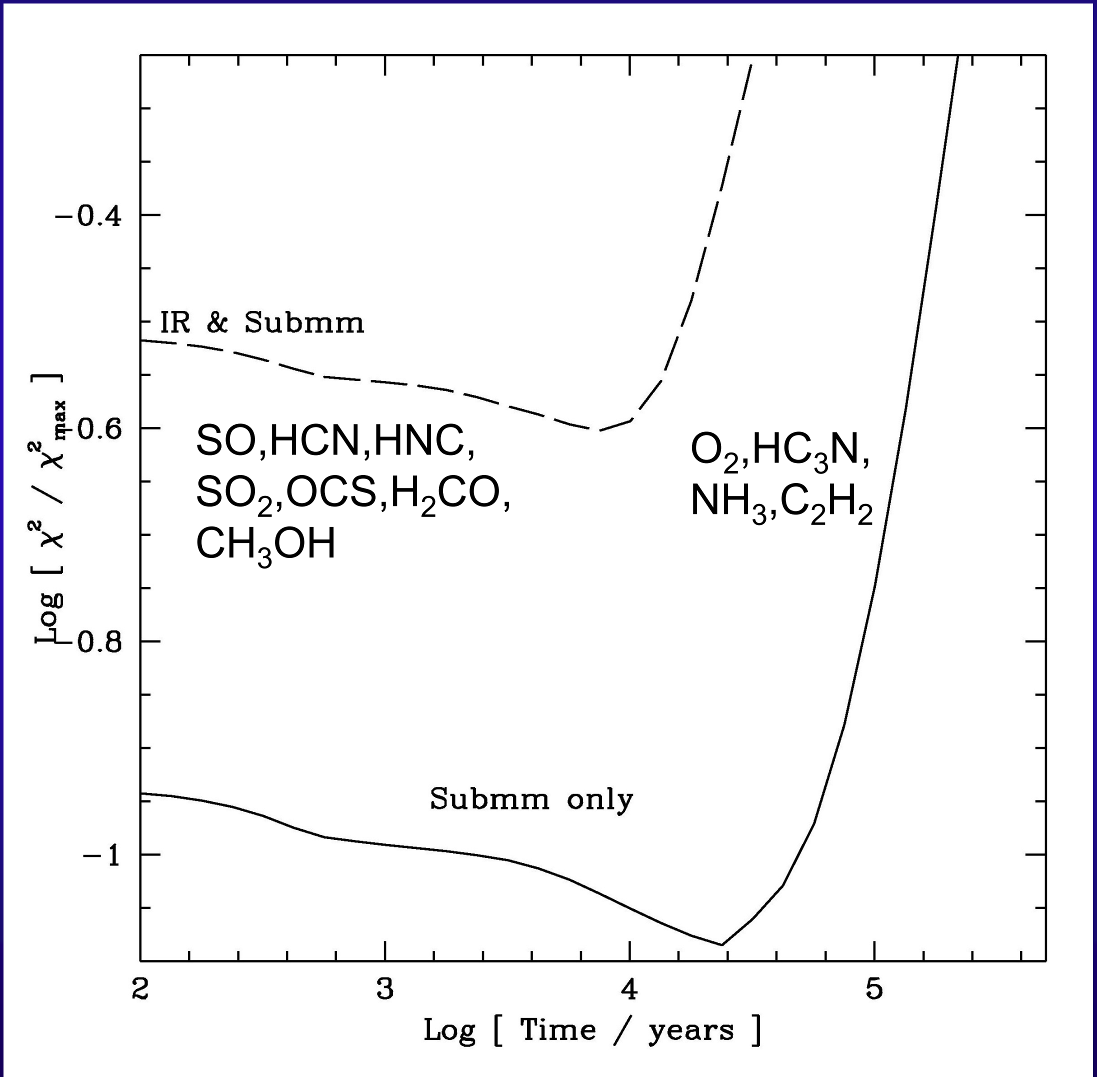
# *AFGL 2591 Chemistry: Base Model*

- Physical structure [ T( r ), n( r ) ] varies w/ position (and time later)
- Solve time-dependent chemistry in this structure
- Treat photo-processes (including UV & x-rays)
- Initial conditions and desorption (0-th order) parameterized to aid in gross understanding
  - Grain surface ad/desorption included heuristically via evaporation at 100K: e.g., *H2O, CO2, H2S, H2CO, CH3OH*
  - Initial conditions loosely based on Charnley hot-core
  - Laboratory-based multi-step desorption included later

# *Age-Dating AFGL 2591*

Determine $\chi^2$ for all species as function of time

Near simultaneous agreement for t ~ 3 x $10^4$ years



# *Some Molecules Toward GL2591*

***Molecule*** ***Inferred Properties***

$CO$

$CO_2$

$O_2$

$HCN$

$CH_4$

$C_2H_2$

$CS$

$SO_2$

$H_2O$

& >21 other species

MASS

AGE

X-RAYS

HIGH T, n

ROLE OF ICES/GRAINS

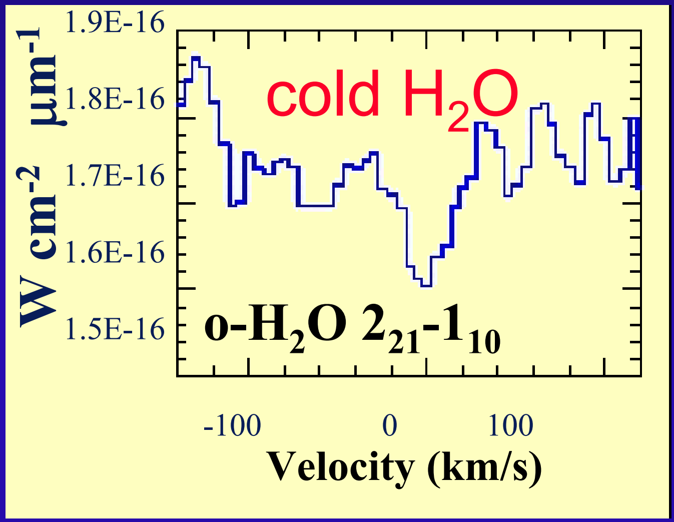
n( r, t ), EVOLUTION

# *Water*

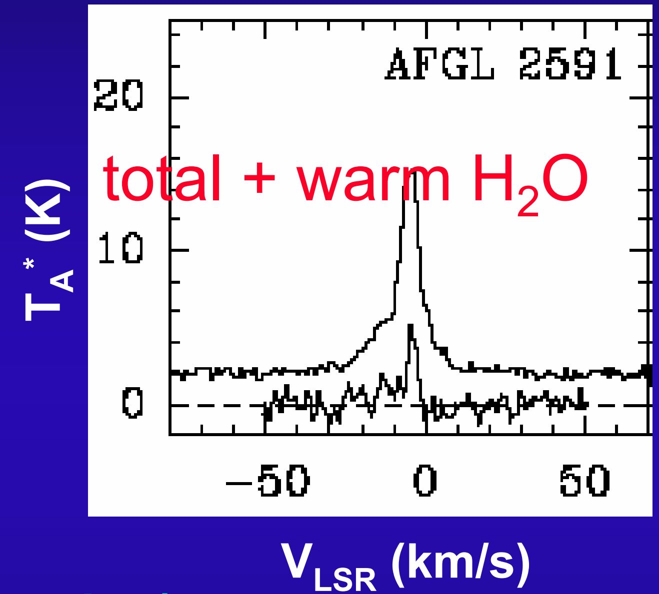
- Water is astrophysically and astrochemically important
- Significant recent (ISO, SWAS) and upcoming (Herschel) data
- Wide range of excitable levels (good test of structure integrated along source)
- Significantly ad/desorbed – may trap other species in pores (good surface / gas interface probe)

# *Water Observations: AFGL 2591*

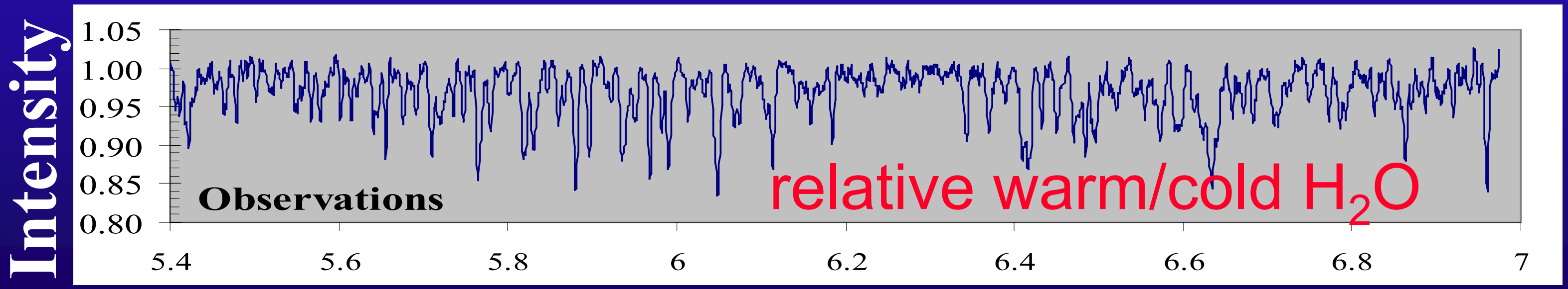
## ISO-LWS (108μm)




## SWAS 557 GHz




## ISO-SWS (6μm absorption)



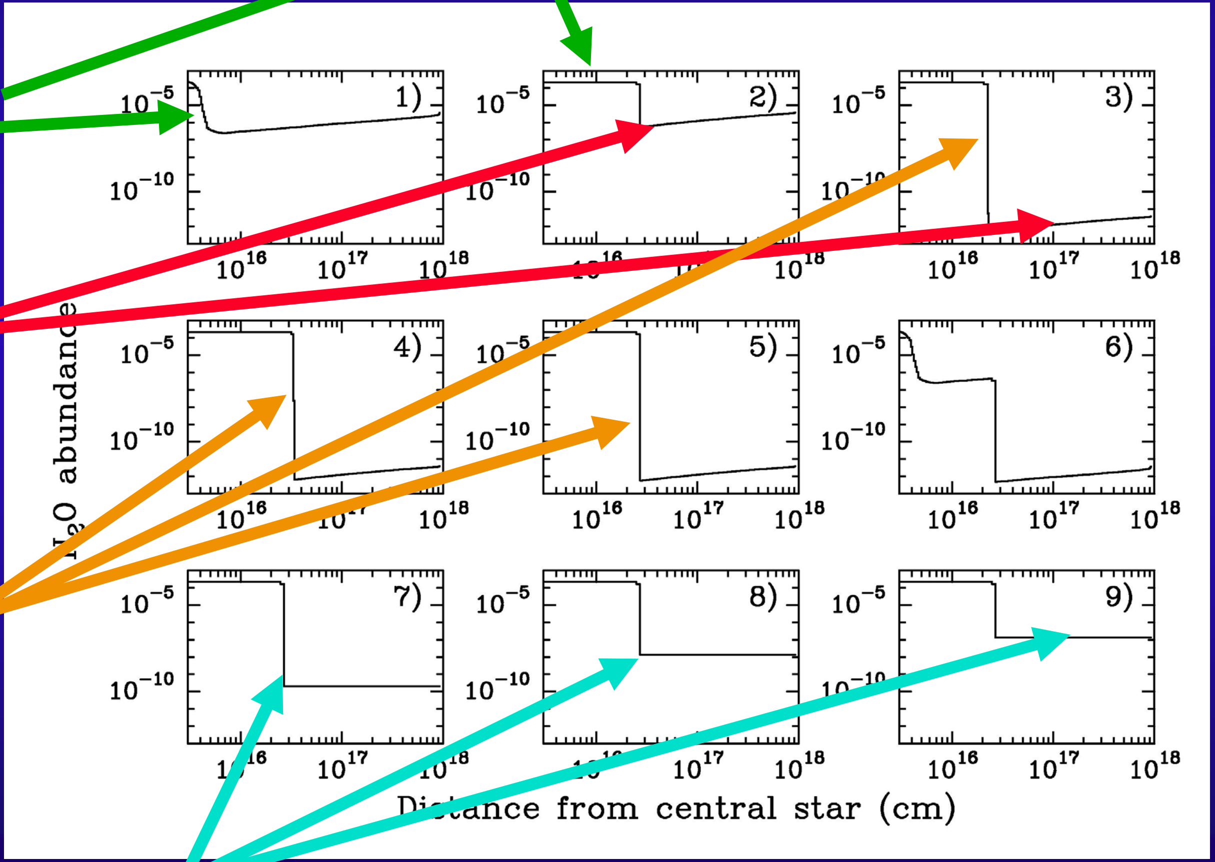

Boonman et al. 2003

# Water Scenarios Tested: Parameterization

(no) ice evaporation for T ~ 100K

(no) freeze out of $H_2O$ for T < 100K

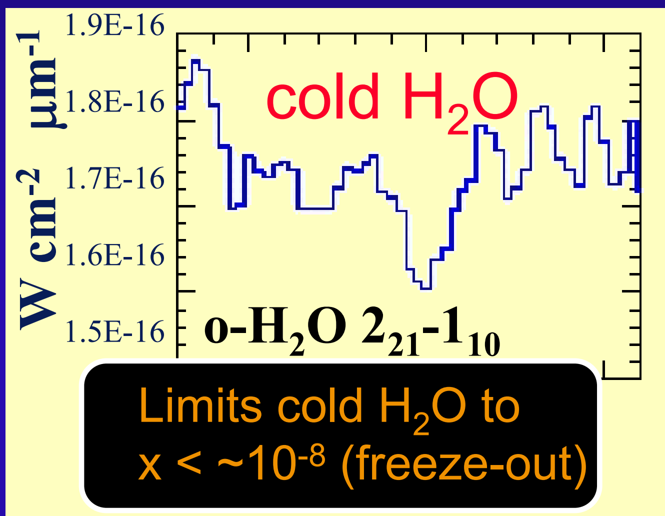
evaporation temp




amount of cold gas $H_2O$

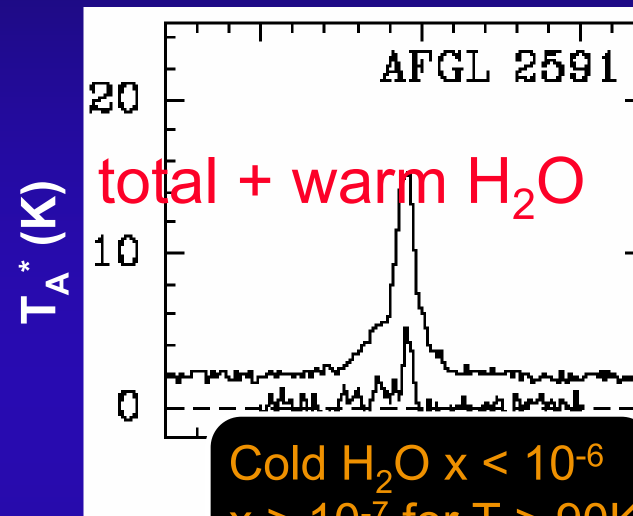
# *Water Observations: AFGL 2591*

**ISO-LWS (108μm)**



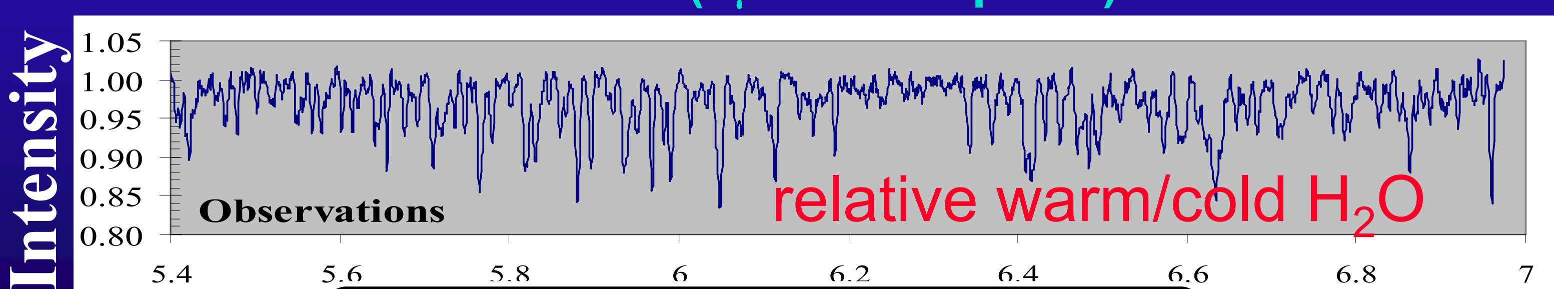

Limits cold $H_2O$ to
$x < \sim 10^{-8}$ (freeze-out)

**SWAS 557 GHz**




Cold $H_2O$ $x < 10^{-6}$
$x > 10^{-7}$ for $T > 90K$
Tevap > 90K

**ISO-SWS (6μm absorption)**




$x_{warm} \sim 2 \times 10^{-4}$, $x_{cold} < 10^{-8}$, $T \sim 100K$

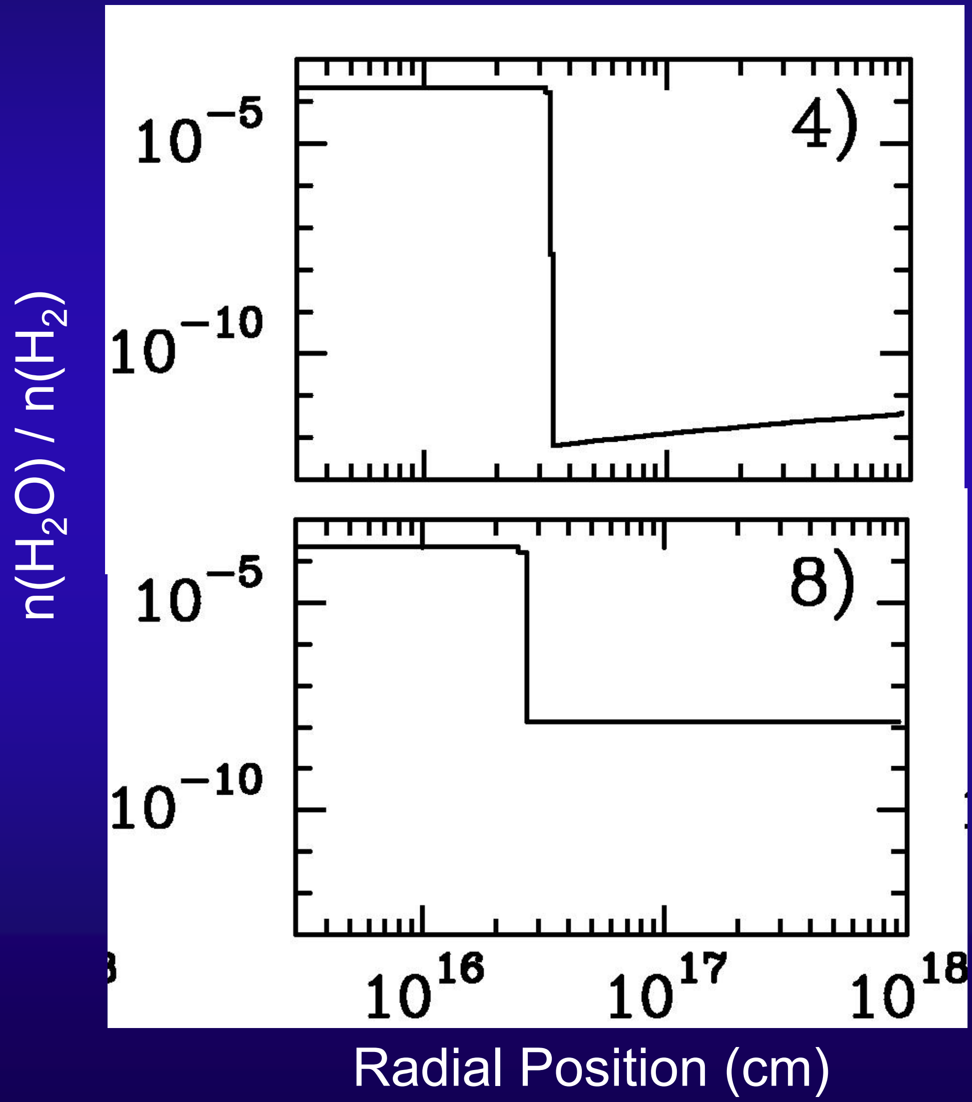
Boonman et al. 2003

# *Best-fit Water Scenarios*

Two scenarios fit data well

Key points

- -Ice evap (>90-100K)
- -Freeze out (<90-100K)
  - -r ~ $10^{16-16.5}$ cm
- -Warm $H_2O$ x~$2\times10^{-4}$
- -Cold $H_2O$ x<~$10^{-8}$



# *One Problem: Parameterization*

Parameterization gives us a clue, but does it agree with our micro- physical/chemical understanding?

Q. Can we explain the origin of the parameterized water abundance distribution?

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Parameterization gives us a clue, but does it agree with our micro- physical/chemical understanding?

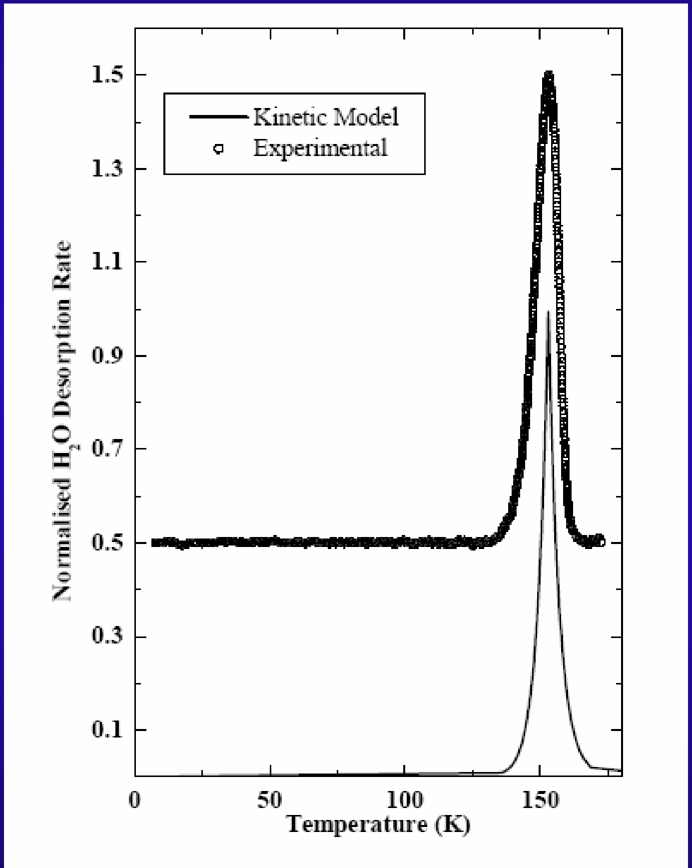
Q. Can we explain the origin of the parameterized water abundance distribution?

A. Yes

# *Laboratory Data to the Rescue*

Temperature-programmed desorption (TPD) data exists for $H_2O$ and $H_2O$ + others *(Fraser et al.; Collings et al.)*

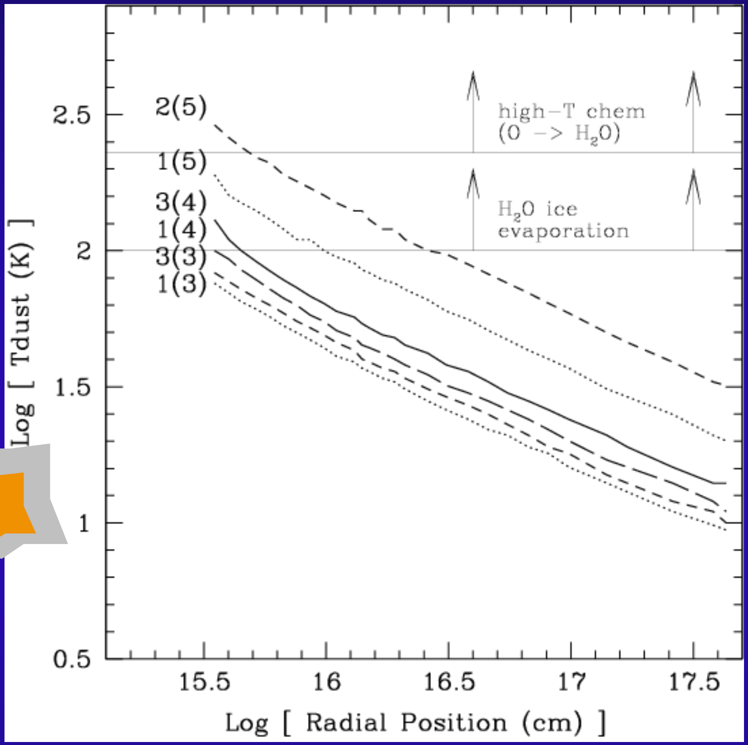
Ability to explicity treat mantle desorption allows us to move away from strictly parameteric description.

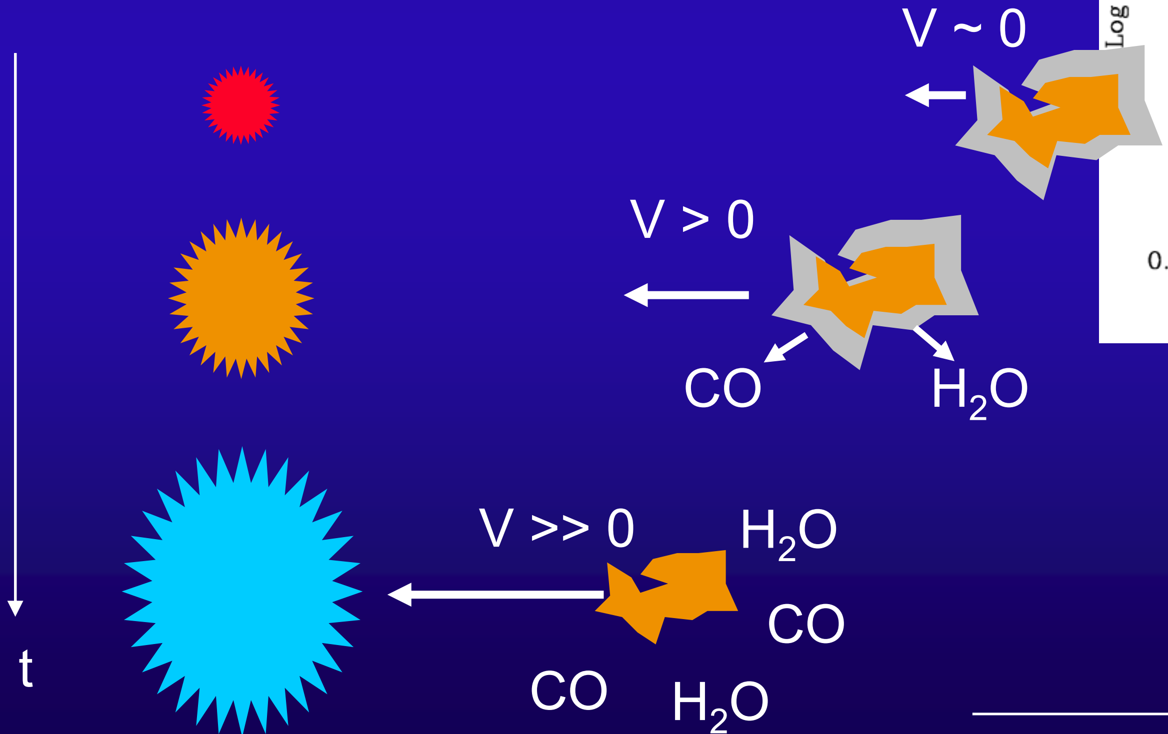



*Fraser et al. (2001)*

# *Explict Source Evolution*

- Envelope collapse *(material inflow from cool/sparse to warm/dense)*
- Stellar evolution $L_*(t)$, $T_*(t)$, $T(r,t)$ *(McKee & Tan 2003)*
- Incorporate ad/desorption

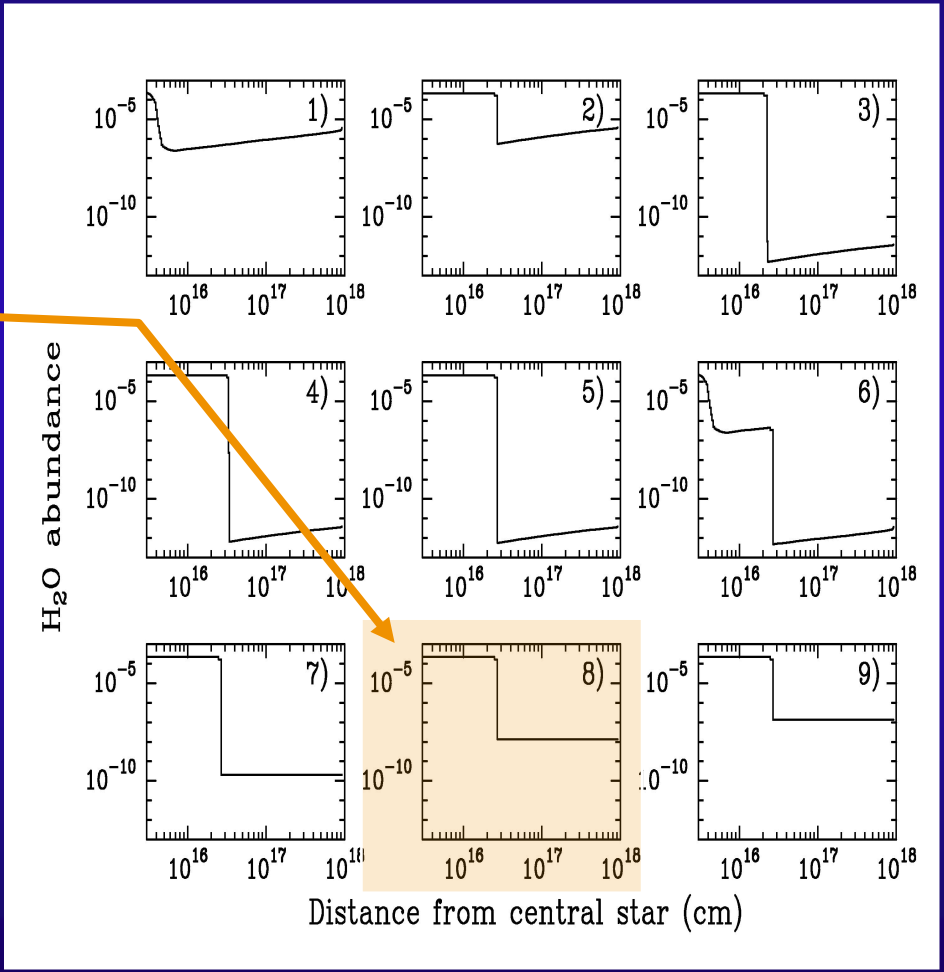



Mantles "naturally" evaporate as material infalls to warming core

# *Parametric Water Results: Summary*

Water observations lead to 3 constraints




1. $x(H_2O)_{hot} \sim 2 \times 10^{-4}$
2. $x(H_2O)_{cold} < \sim 10^{-8}$
3. "Jump" in $x(H_2O)$ near $r \sim 10^{16\text{-}16.5}$ cm

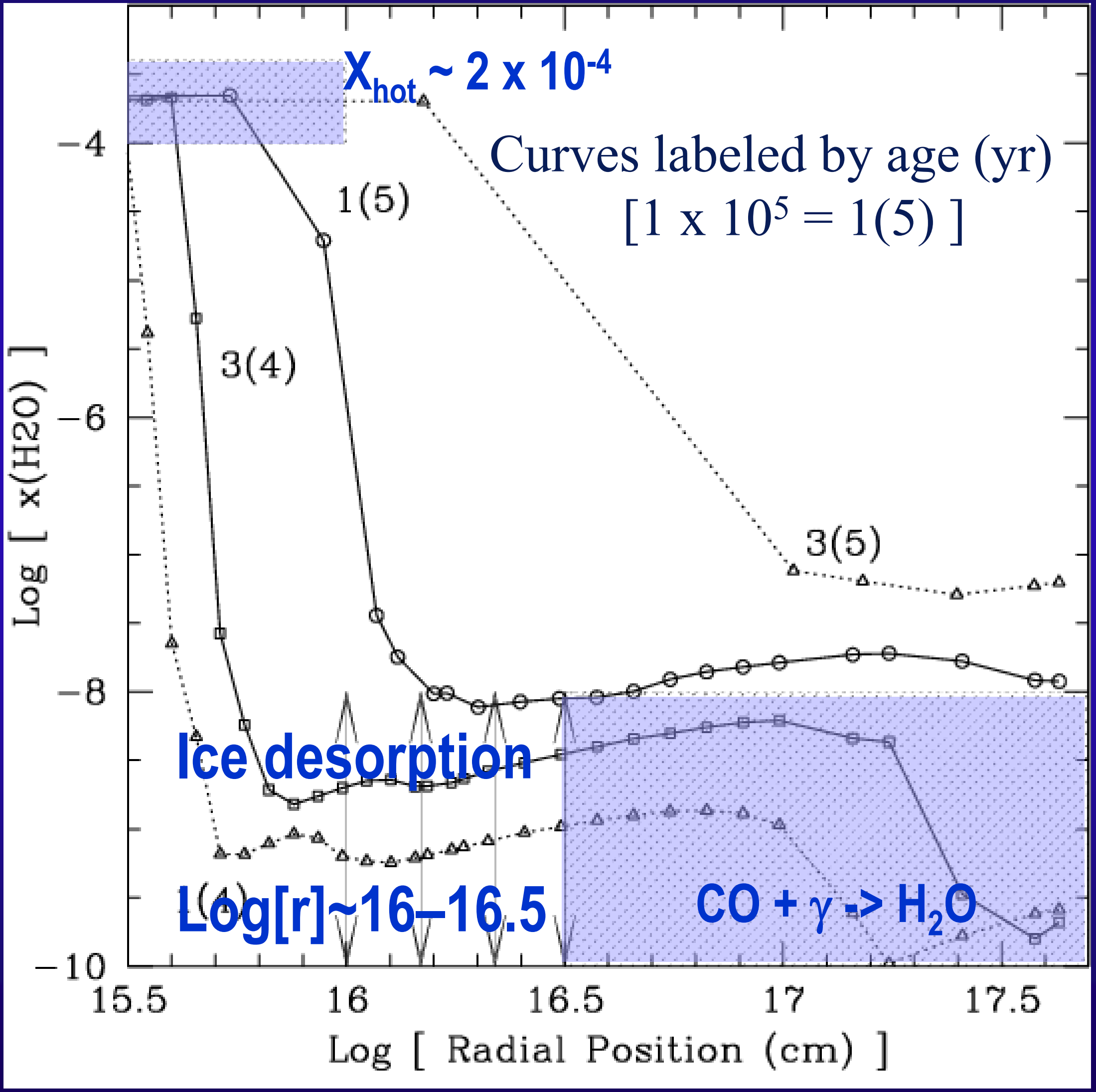
# *Water Abundance: Non-Parametric*

Previous constraints

- ✓$x_{hot}$ ~ 2 x $10^{-4}$
- ✓$x_{cold}$ < ~ $10^{-8}$
- ✓r(des) ~ $10^{16-16.5}$

Evaporation in an evolving source w/ desorption naturally explains x( r )

"time" since YSO formation!

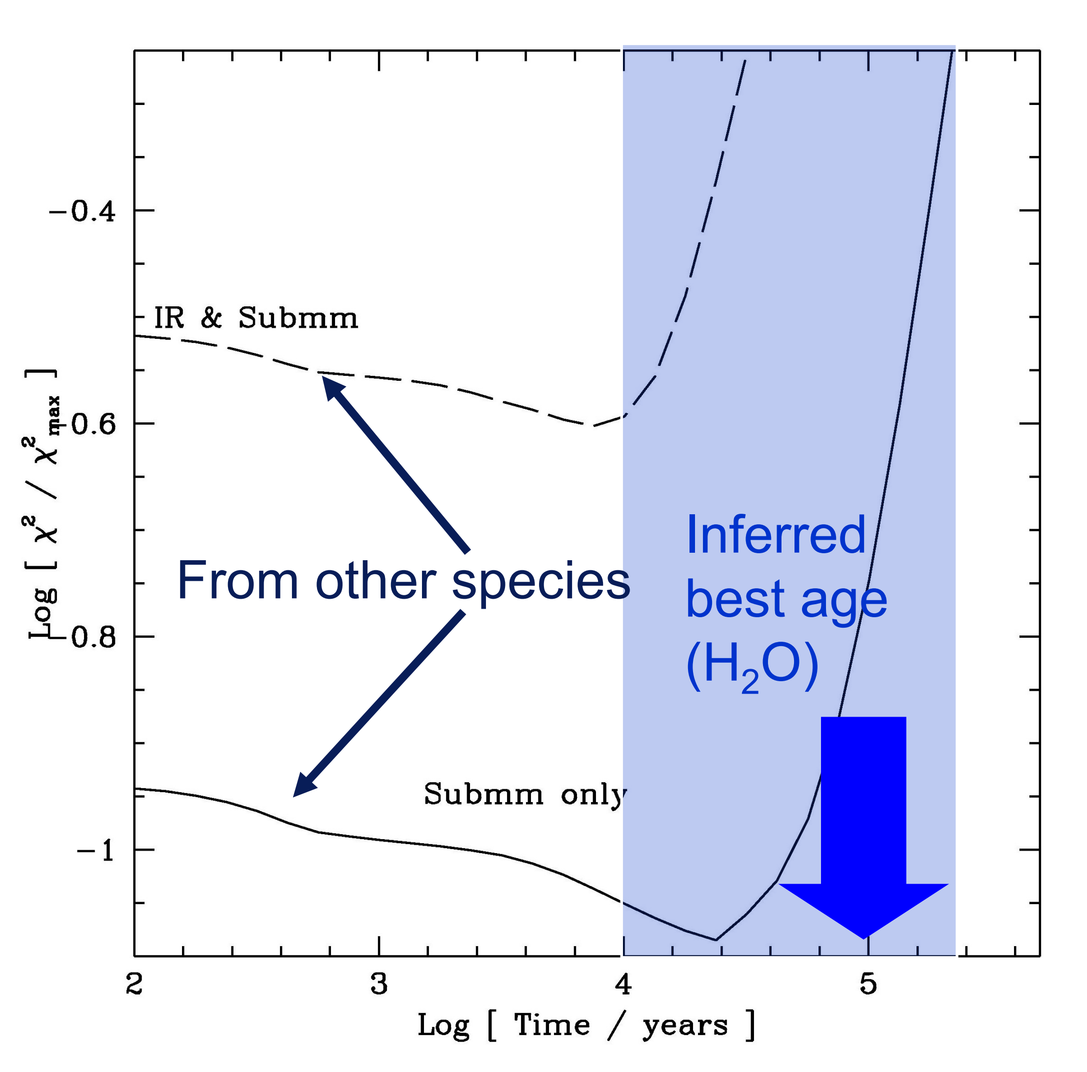



*Doty et al. 2006*

# *Evolution of AFGL 2591: Summary*

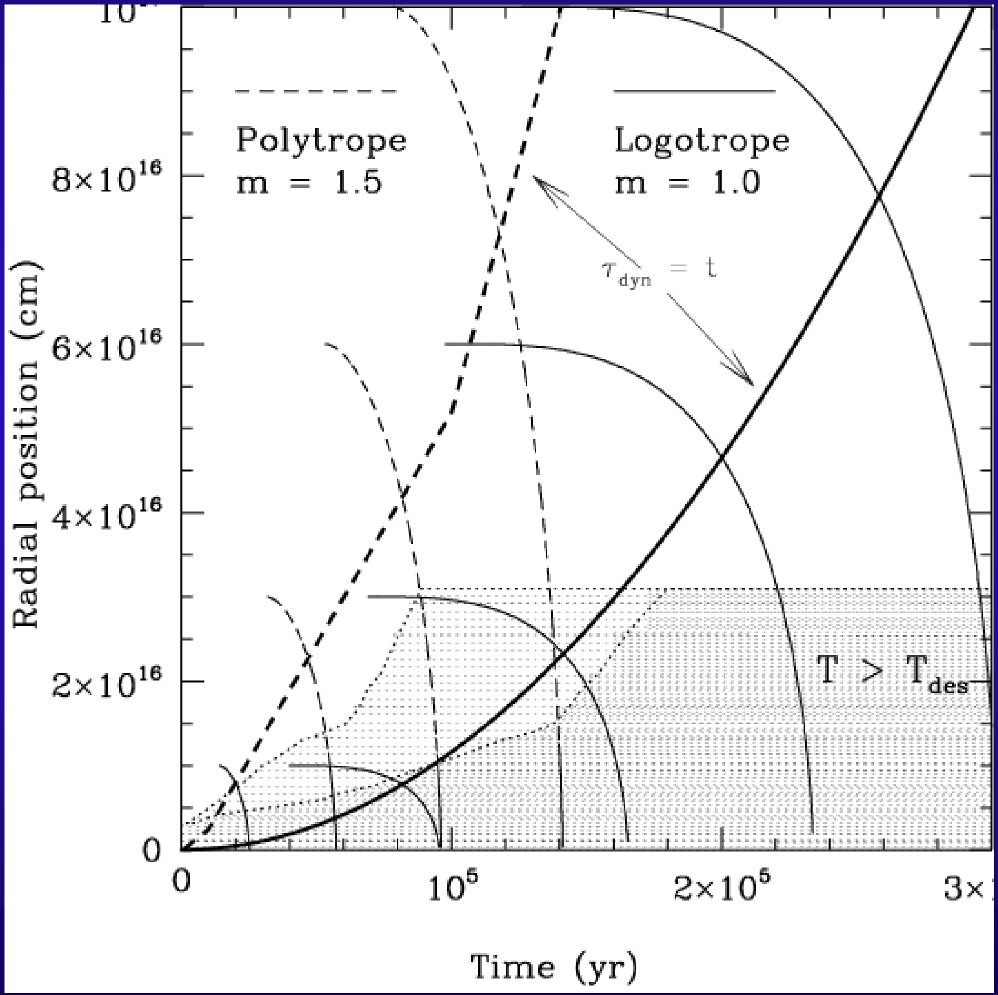
Evaporation in an evolving source w/ desorption naturally explains x( r )

Confirms
t ~ 3-10x$10^4$ years



# *Fast Collapse: Consequence*

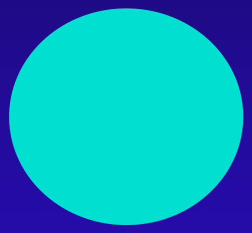
- Gas/dust parcels spend most time ~ static
- Parcels spend little time infalling, and accelerate toward small r quickly
- Hot gas lifetimes (>200AU) ~ $10^4$ yr +/- 0.5 dex



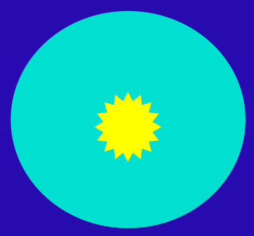

*Doty et al. 2006*

# *Evolutionary Picture?*

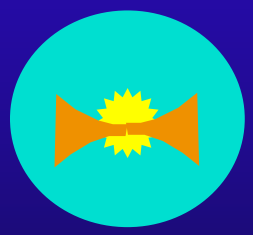
- $t < 10^4$ yr
  - static, cold envelope



- $t < 1 – 8 \times 10^4$ yr
  - ~ static hot core, $r \sim 10^{16}$ cm
  - cold, ~ static envelope



- $t > 1 – 8 \times 10^4$ yr
  - dynamic hot core ($> 2\text{-}3 \times 10^{16}$ cm)
  - cold, ~ static envelope
  - disk?



# *Evolutionary Picture?*

Complex hot chemistry beam-diluted in small central structure (like disk?) → ALMA

( θ ~ 0.25'' at 1 kpc )

- t > 1 – 8 x $10^4$ yr
  - dynamic hot core (> 2-3 x $10^{16}$ cm)
  - cold, ~ static envelope
  - disk?

# *Modeling: Sample Results*

- Goal: understand structure of star-forming regions
- Detailed models reproduce observations of GL2591 and suggest we are not “stupidly wrong”
  - •CO & $H_2O$ produced on/ liberated from grain mantles; high-T HCN, $CH_4$, $C_2H_2$ chemistry; most S solid/ice below 100K

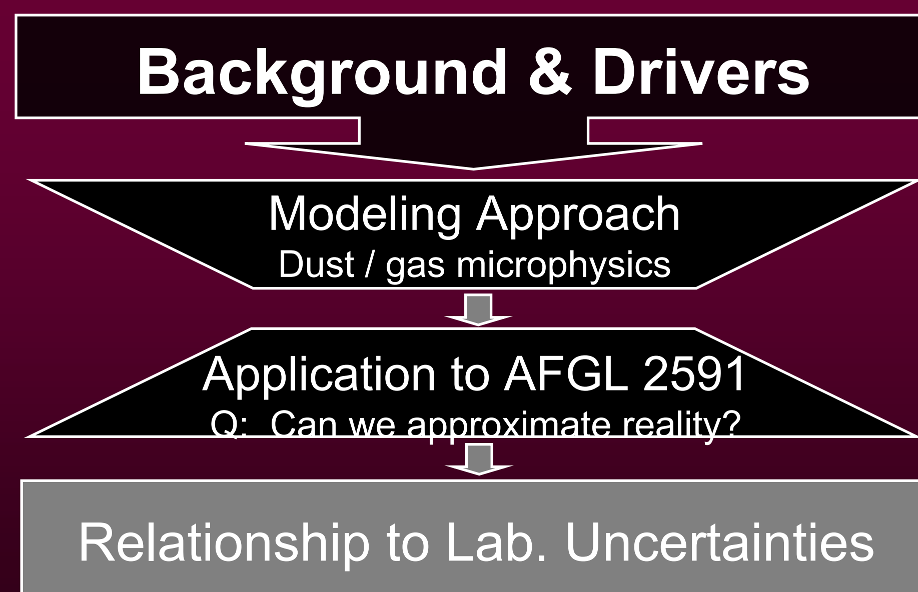
- Astrochemically confirm rapid YSO evolution
- Evolutionary picture of high-mass s.f. emerges

cold envelope -> static hot core -> dynamic hot core

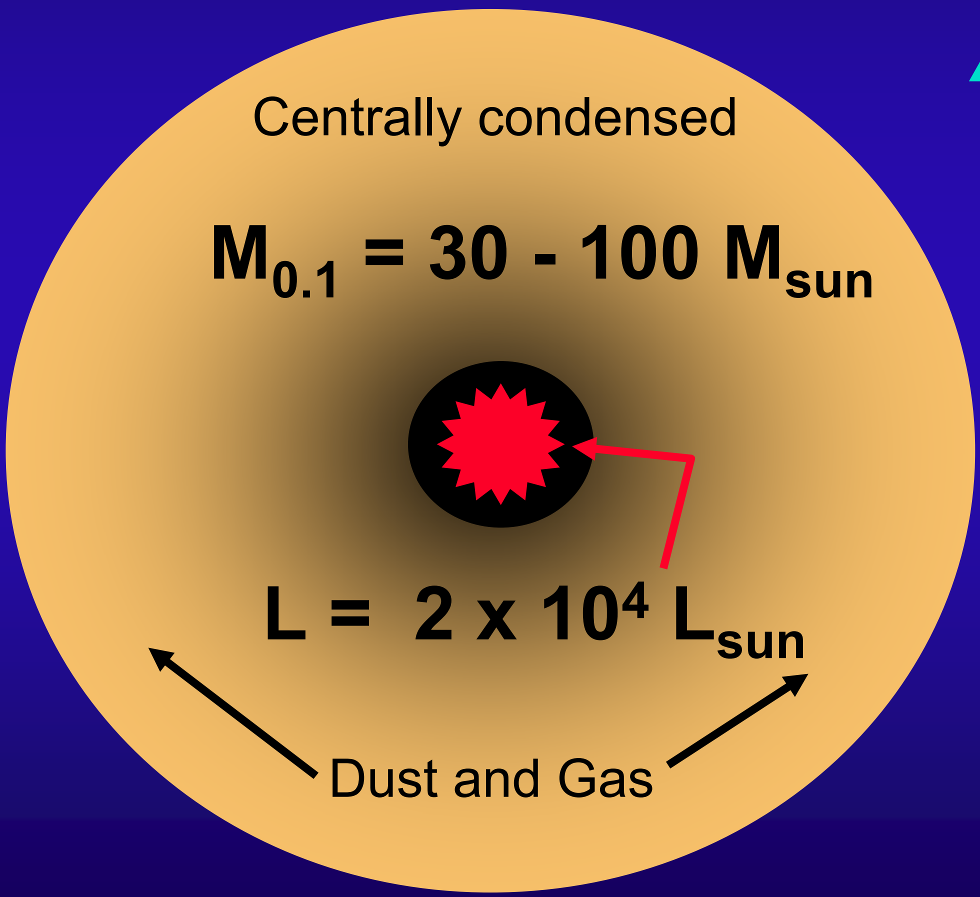
- Residence time in hot gas naturally explains hot core ages ~ $10^4$ yr (beam-diluted in small central structure)
- Sig. complex chemistry on ALMA scales (<0.2’’)

# *Relationship to Lab. Uncertainties*

Q: How good do our input data need to be?



# *Test: HMPO (like AFGL 2591)*

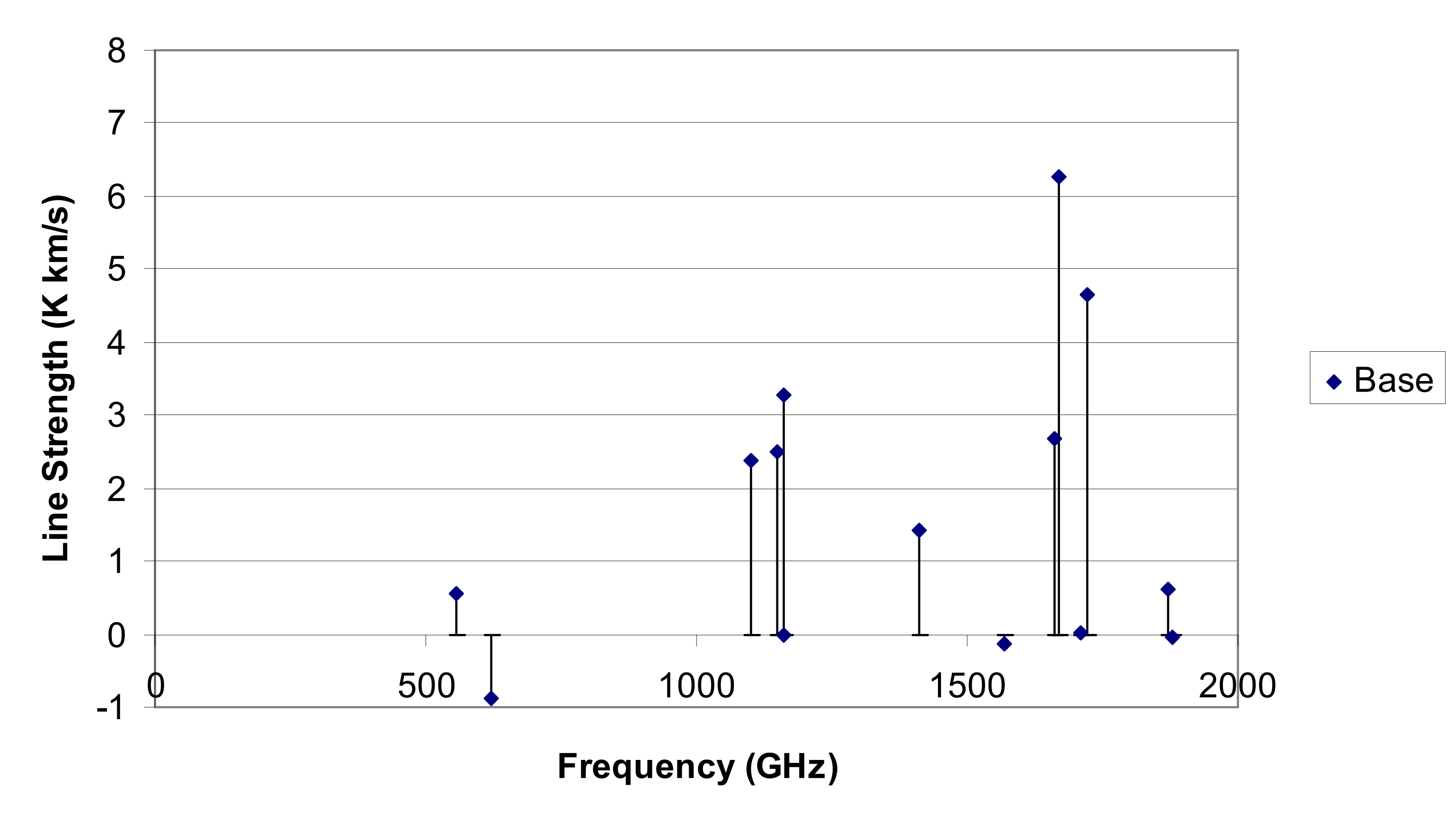



***Approach***

- Consider various physical situations
  - M + 20%
  - Cavity $2r_{in}$
- Consider unceratinty in $A_{ij}$
  - $A_{ij}$ + 20%

*Q: Robust results?*

# *Herschel / HIFI Lines (o-$H_2^{18}O$)*



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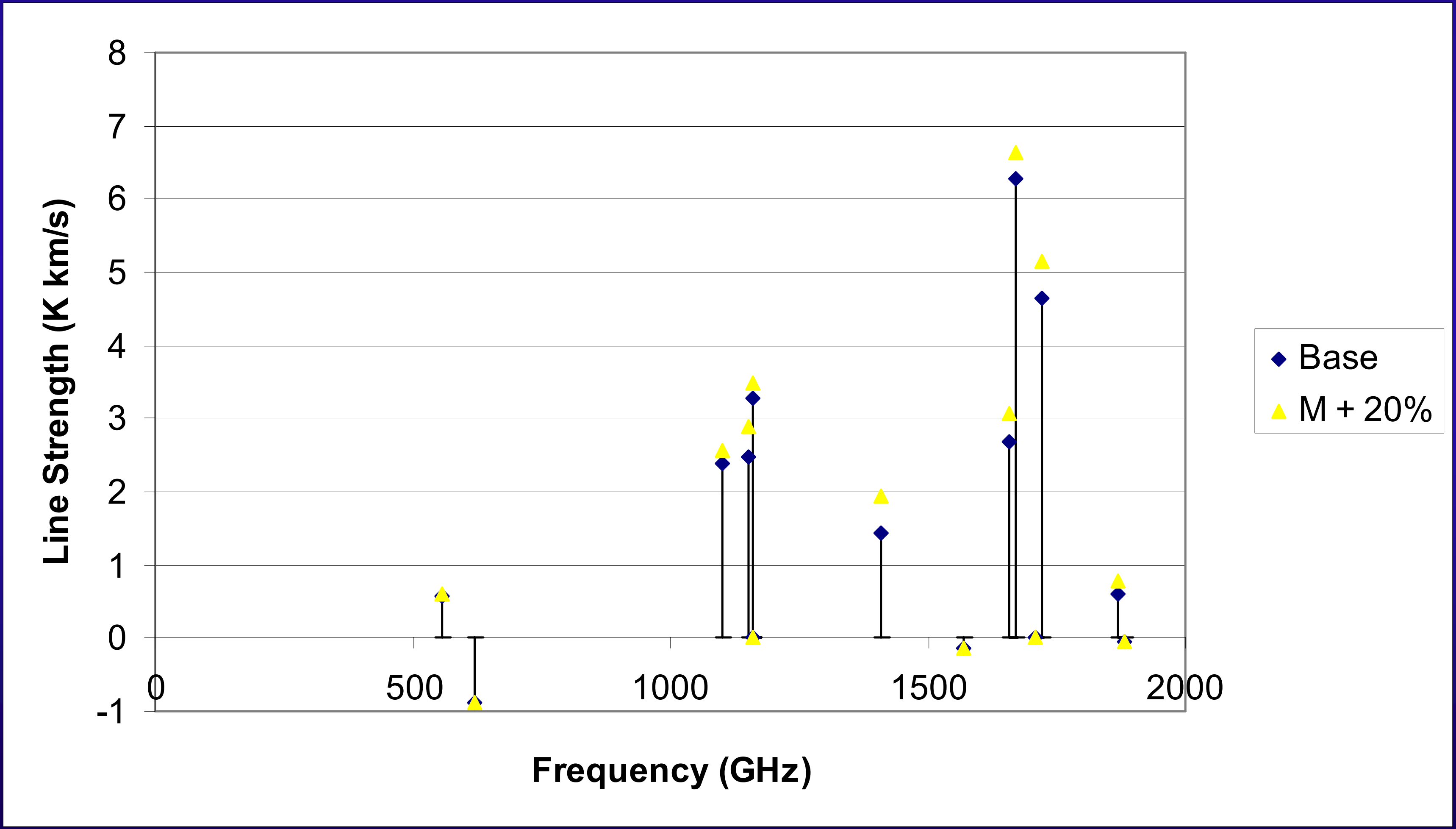

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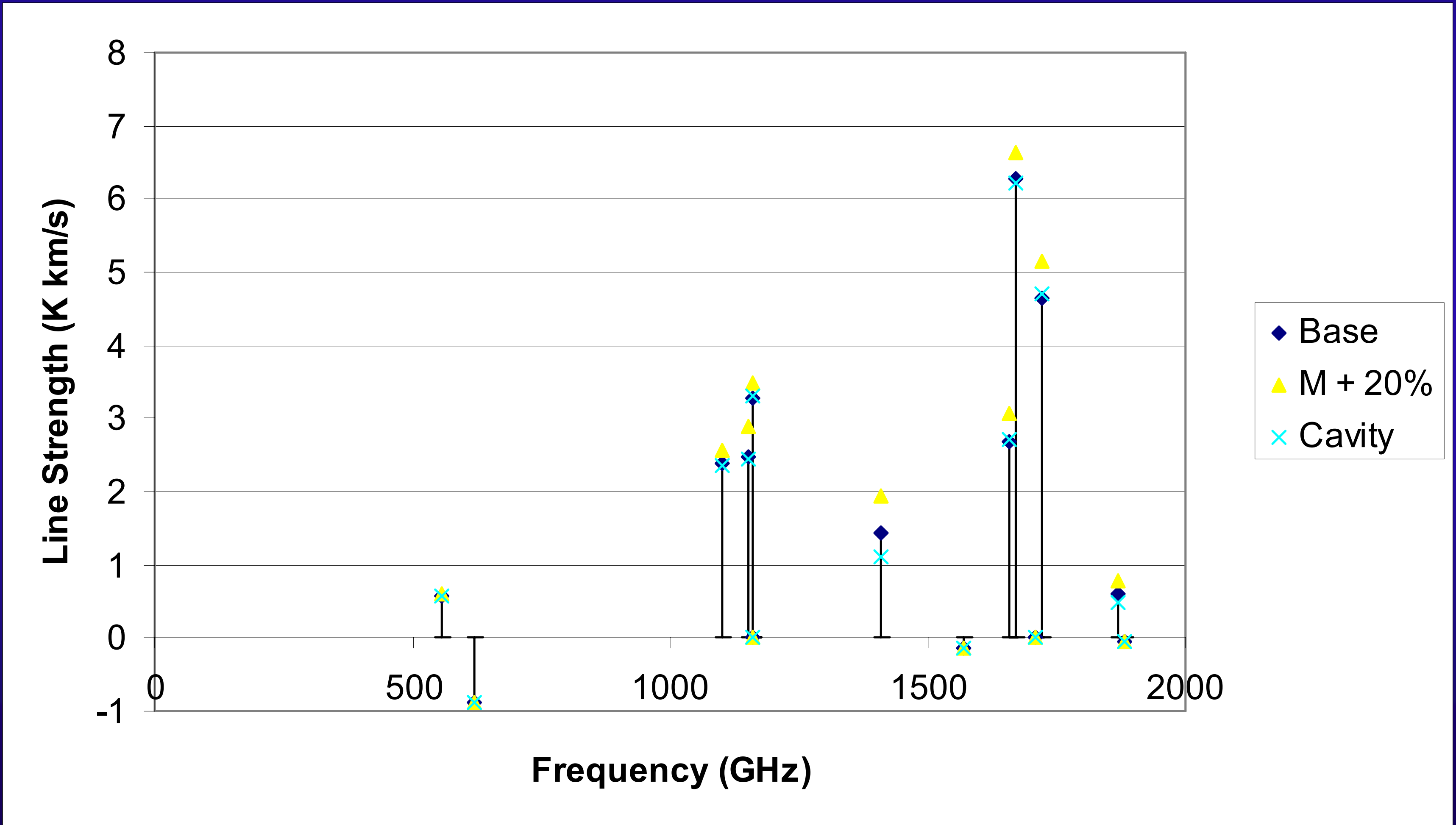

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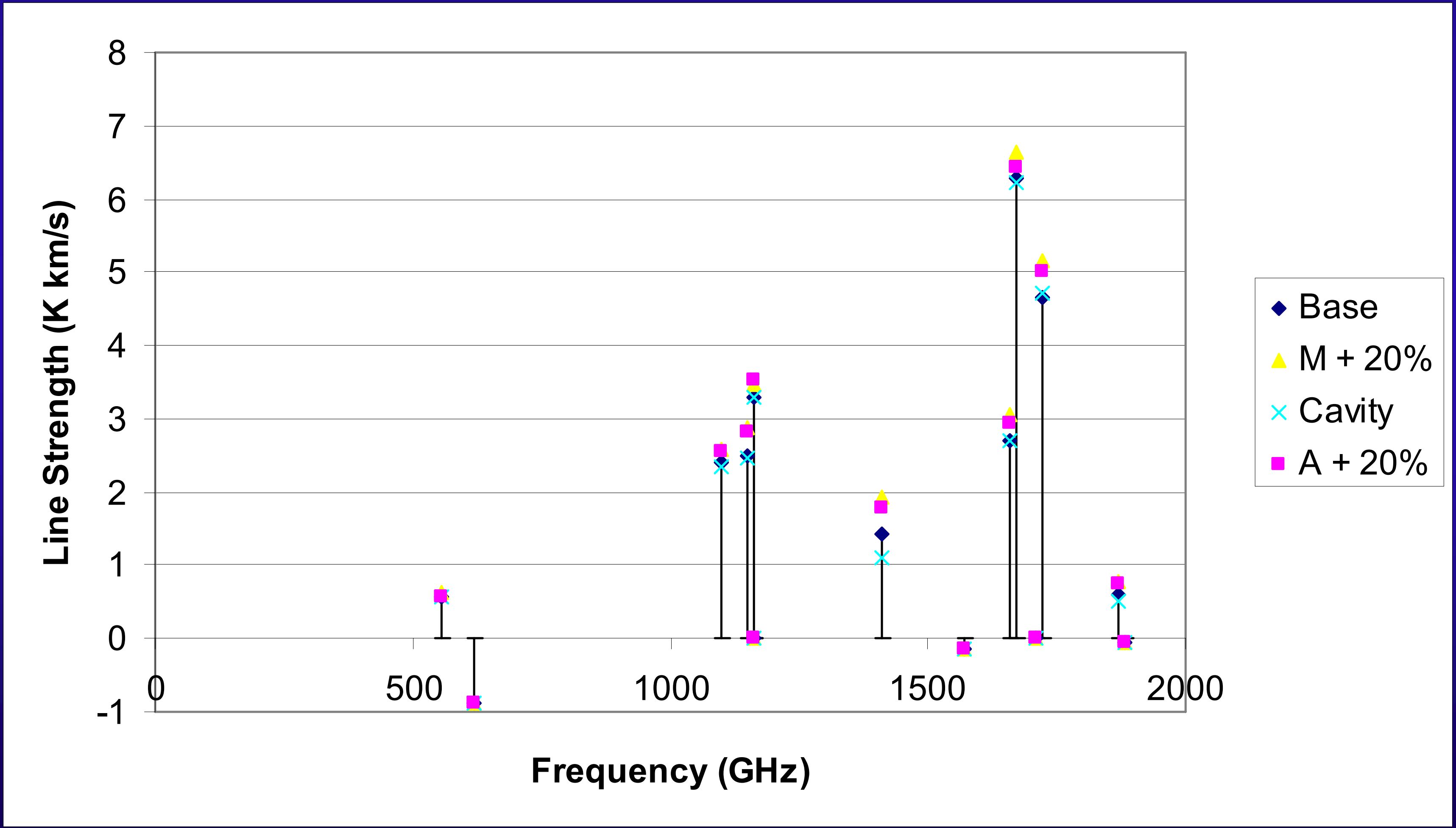

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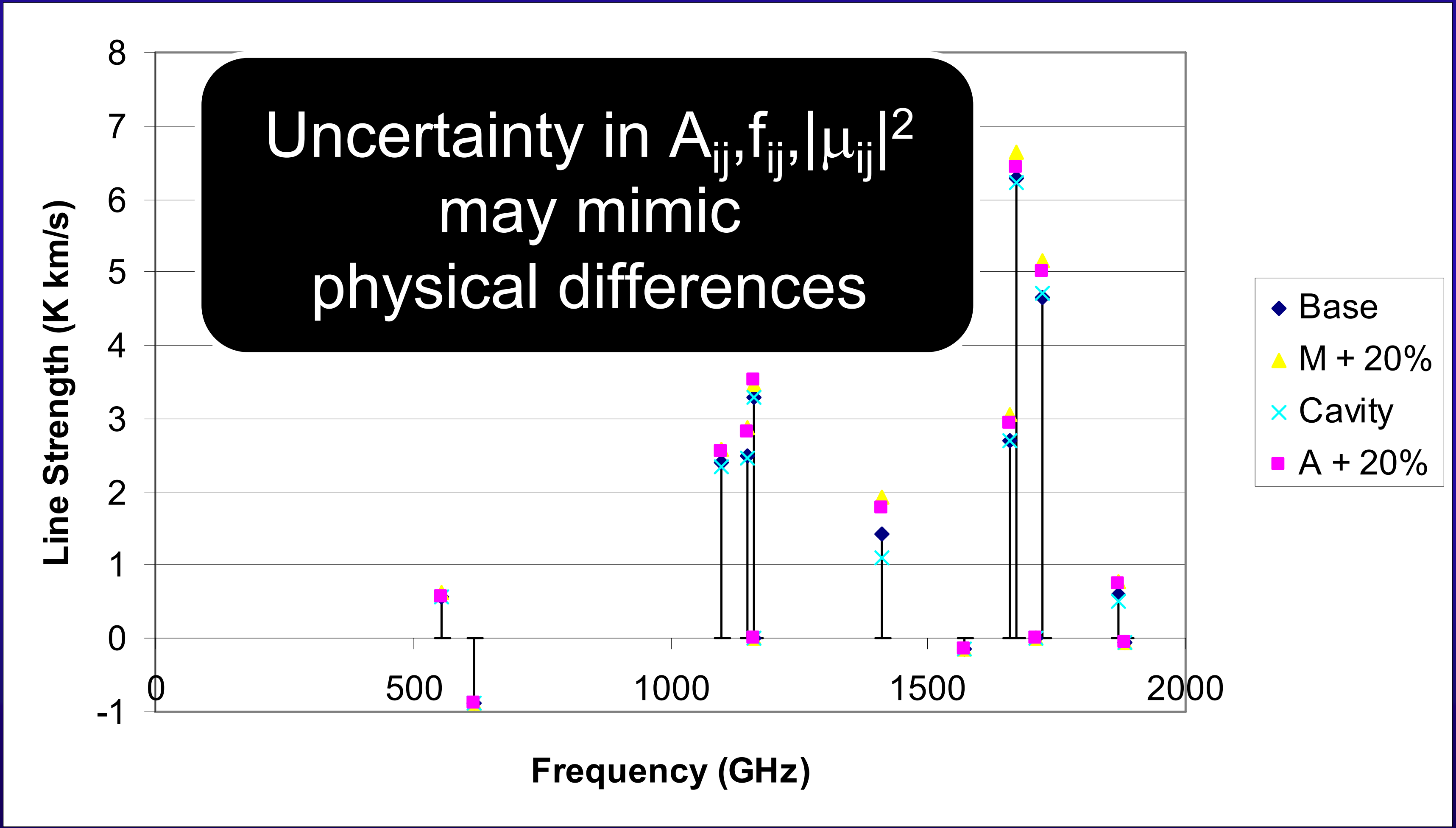
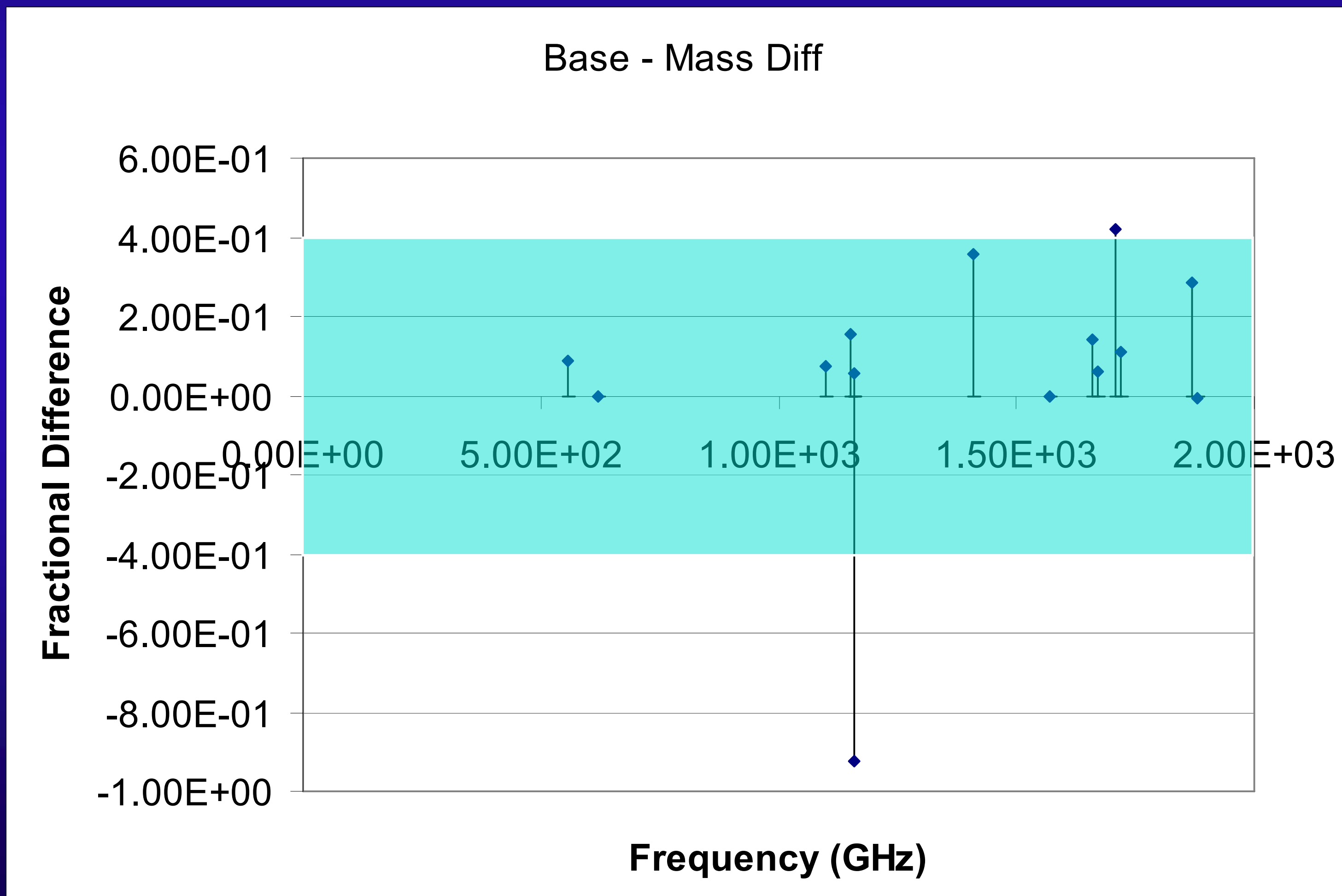


# *Effects of Differences (o-$H_2{}^{18}O$)*

Mass (20%)
~+/- 40%



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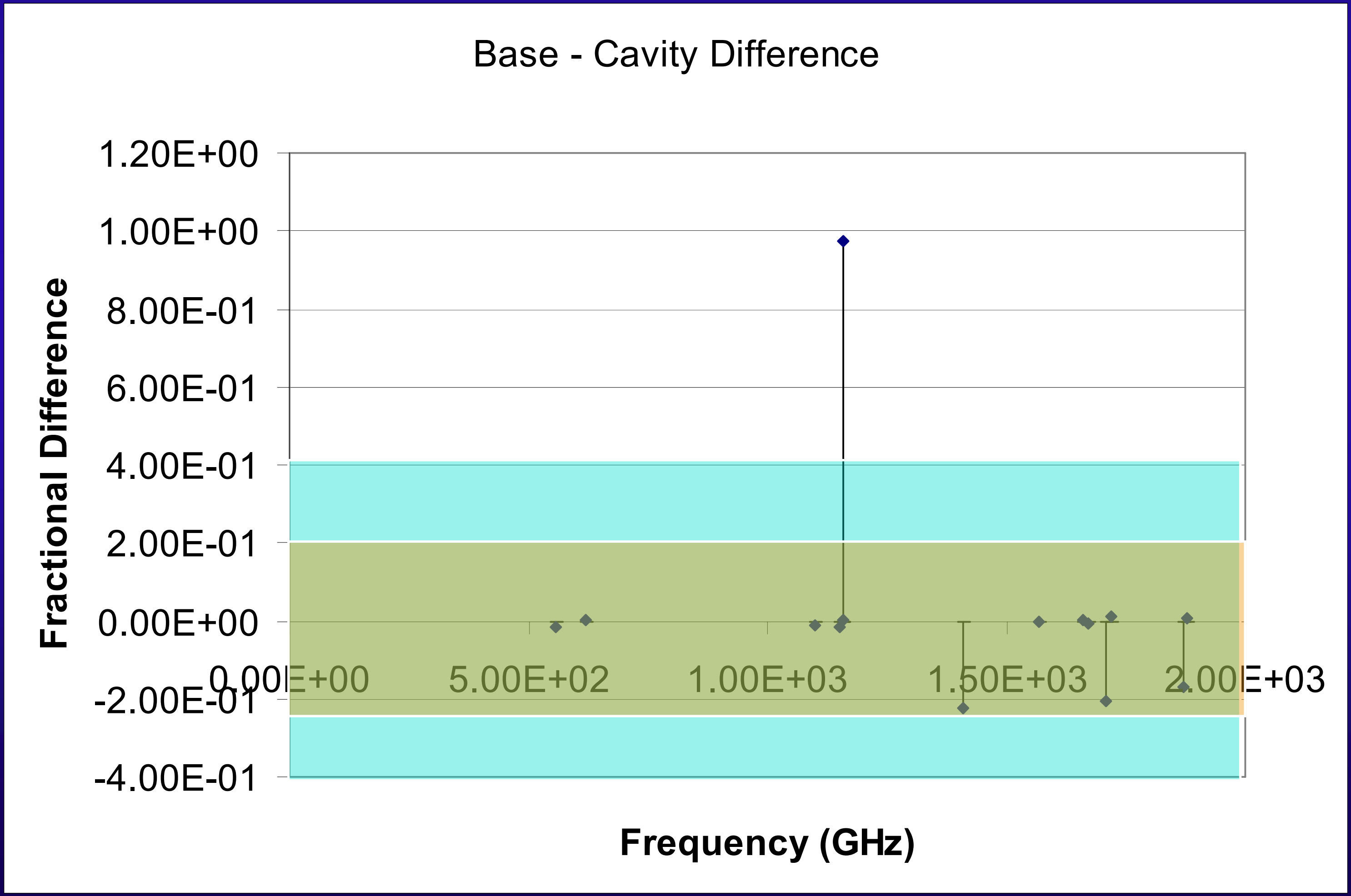
Cavity (2r)
~+/- 20%



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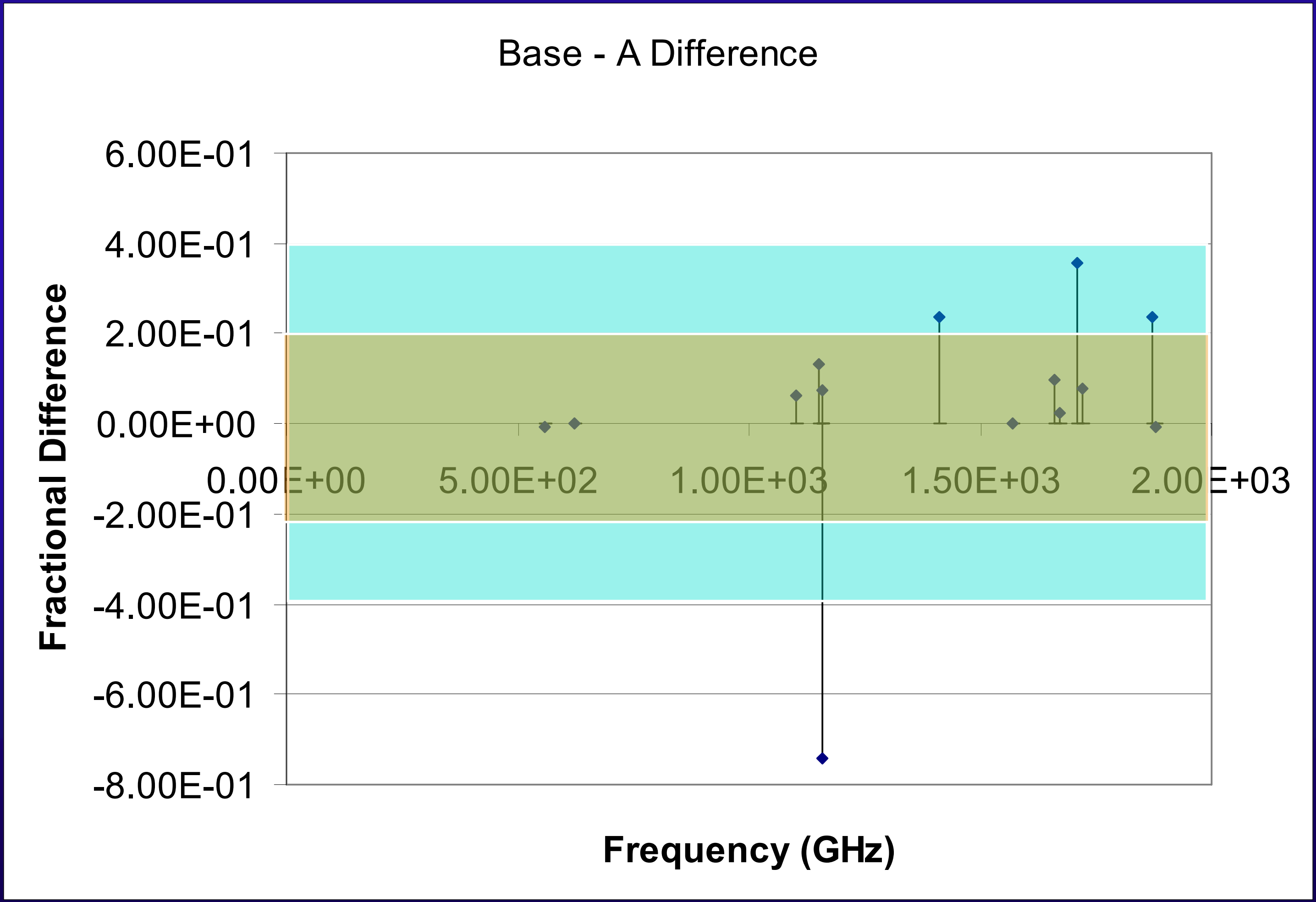
Mass (20%)
~+/- 40%

Cavity (2r)
~+/- 20%

$A_{ij}$ (20%)
~+/- 40%



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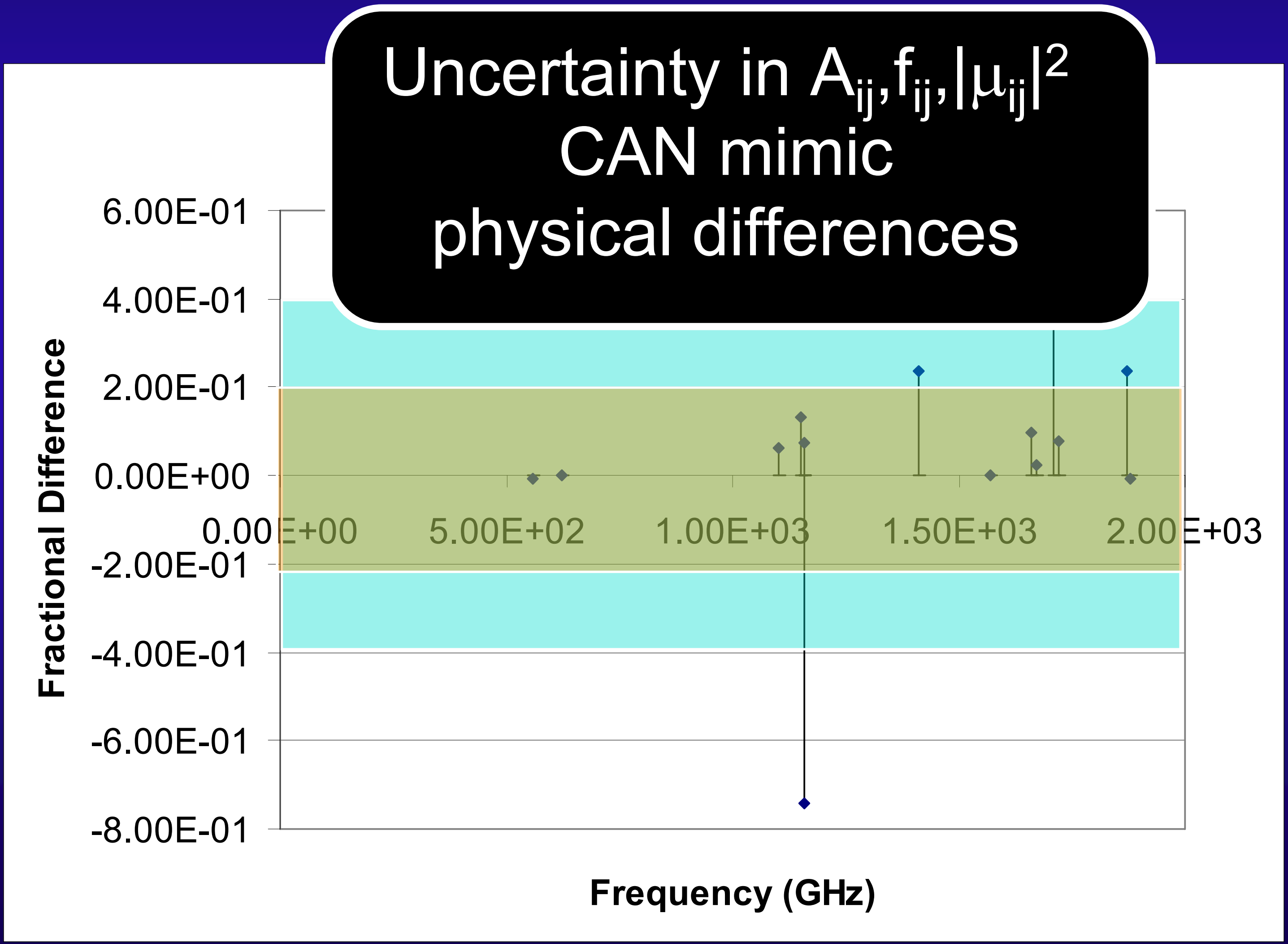
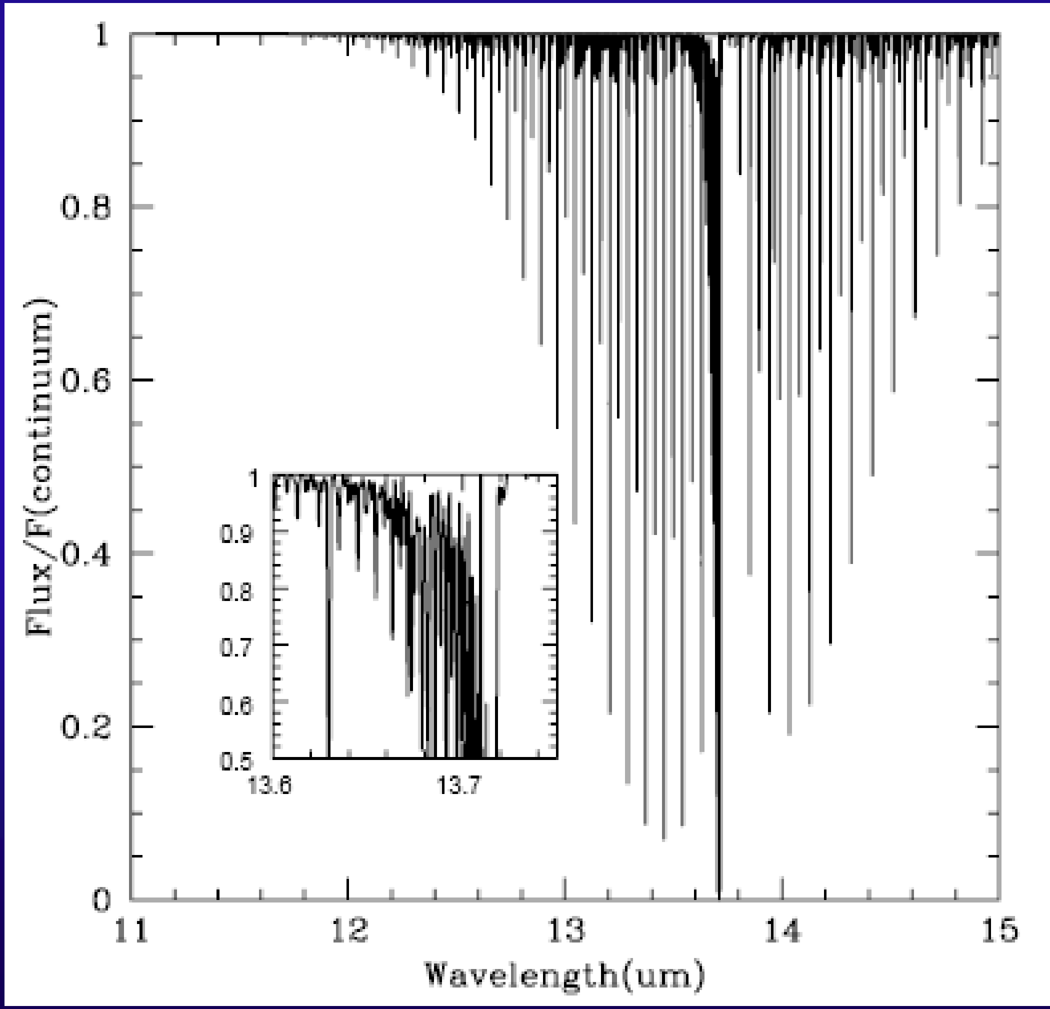


# *SOFIA / EXES Absorption ($C_2H_2$)*

(Ro)Vibrational line absorption at R ~ $10^5$ provides significant constraints on n( r ), T( r ), x( r )

Simulated spectrum toward AFGL 2591



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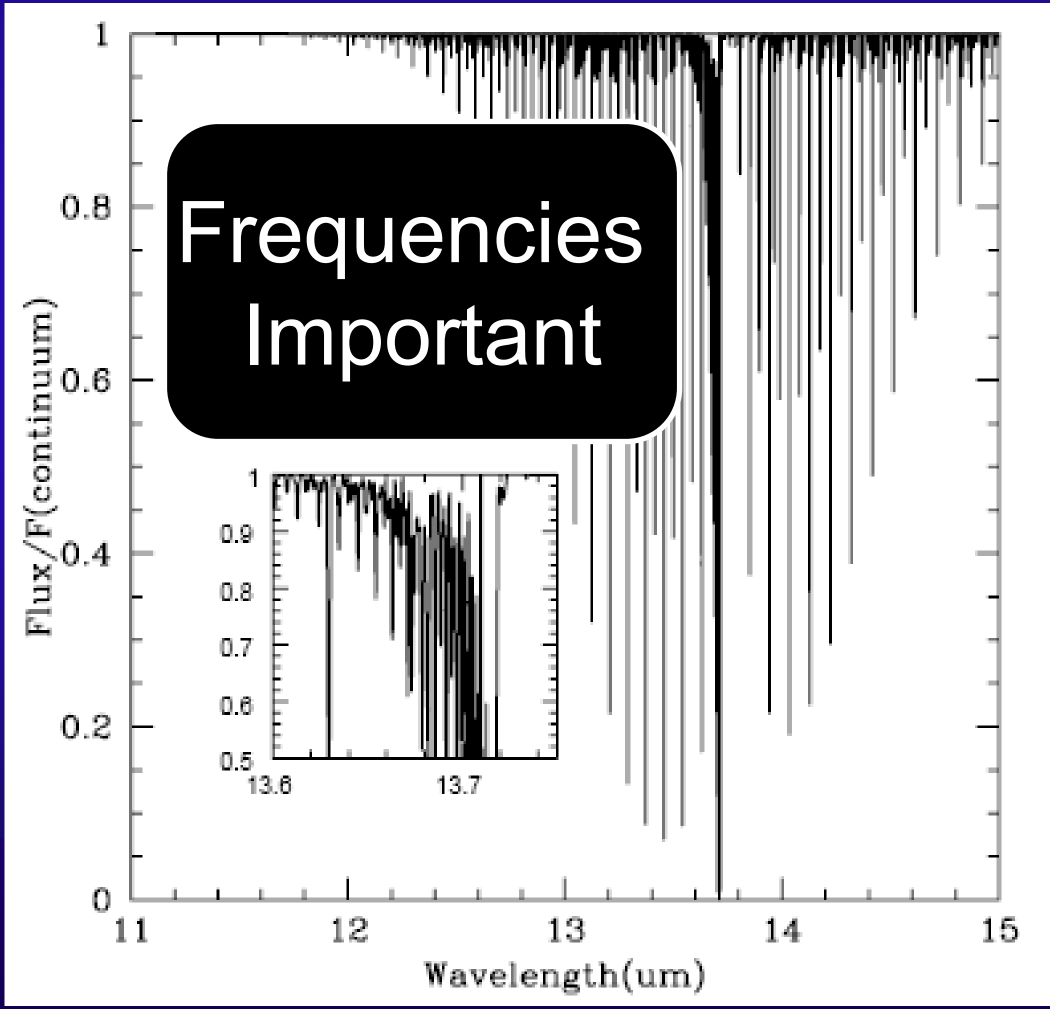
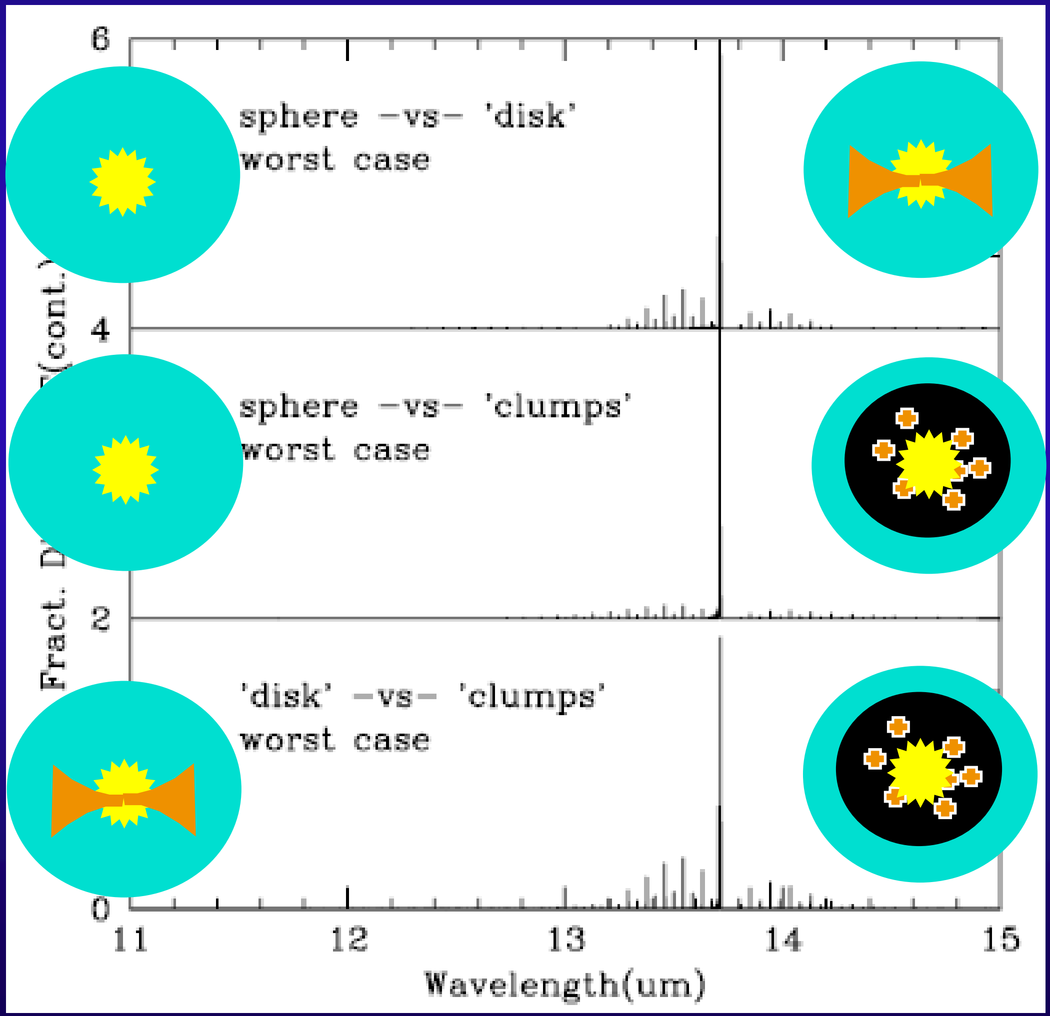


# *SOFIA / EXES Absorption ($C_2H_2$)*

(Ro)Vibrational lines can probe structural differences between sphere, disk, and clumps – even for same N, and $n_{avg}$( r )!

$\Delta F/F_{avg}$ ~ 0.1 – 0.3

$\Delta F/F_{max}$ ~ 30

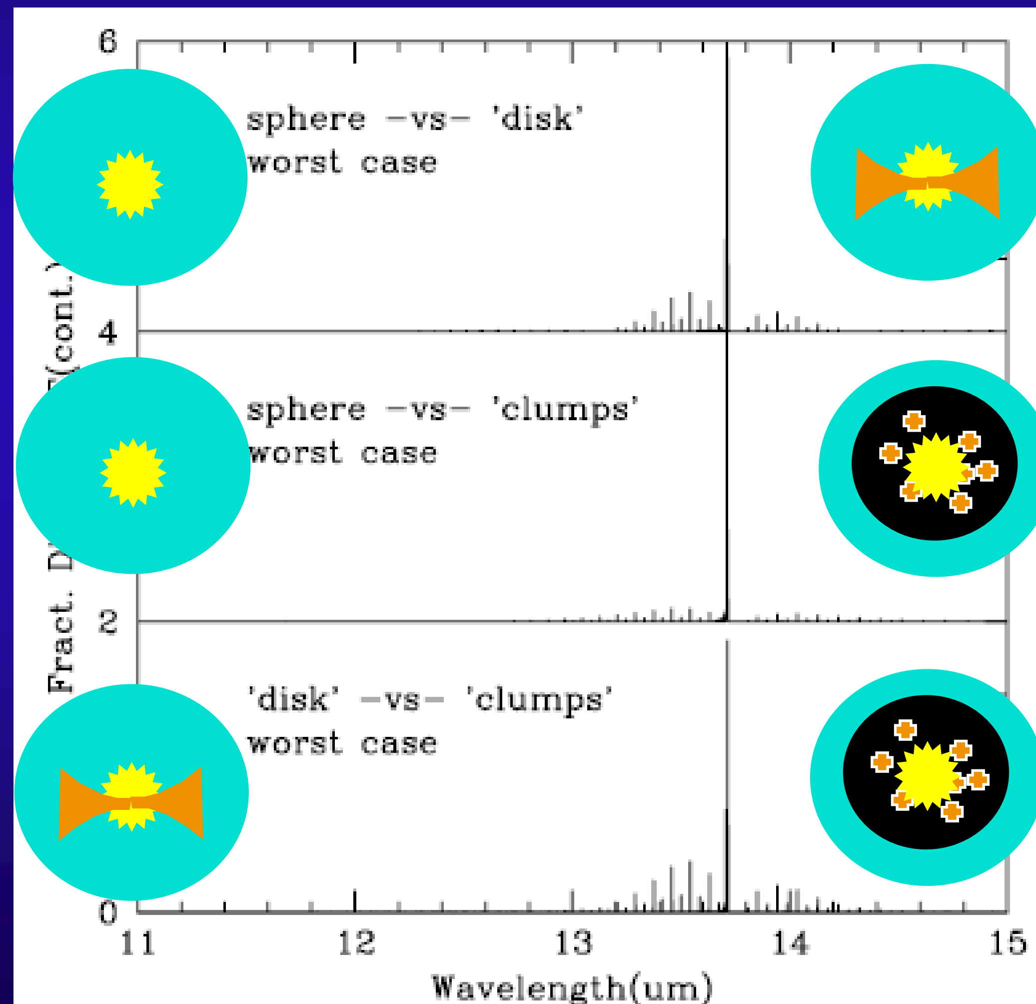


# *SOFIA / EXES Absorption ($C_2H_2$)*

(Ro)Vibrational lines very useful
But need
$\Delta A_{ij}/A_{ij} < \sim 0.2$

same N, and $n_{avg}( r )$!

$\Delta F/F_{avg} \sim 0.1 – 0.3$
$\Delta F/F_{max} \sim 30$



# Conclusions

***Fight the Good Fight…***

- We "have a clue" re: relevant physical and chemical processes in star-forming regions
- Detailed source modeling can yield source prop.
  - FIR/submm rotational lines (T < few hundred K)
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- Outputs are only as good as inputs
  - 20% uncertainties in $A_{ij}$ lead to physical differences (e.g. $\Delta M \sim 20\%$ ; geometry)
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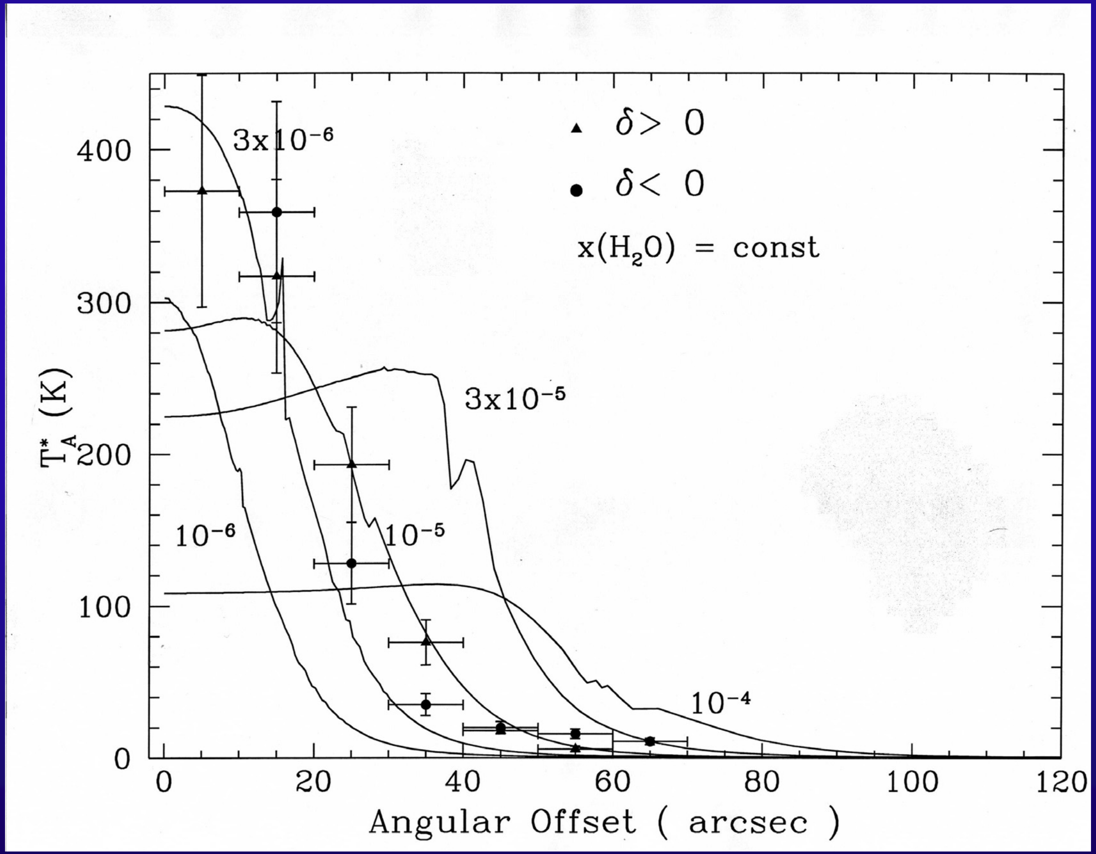
# *Water Masing in Orion*

183 GHz masing observed to IRC2

Line strengths can be re-produced

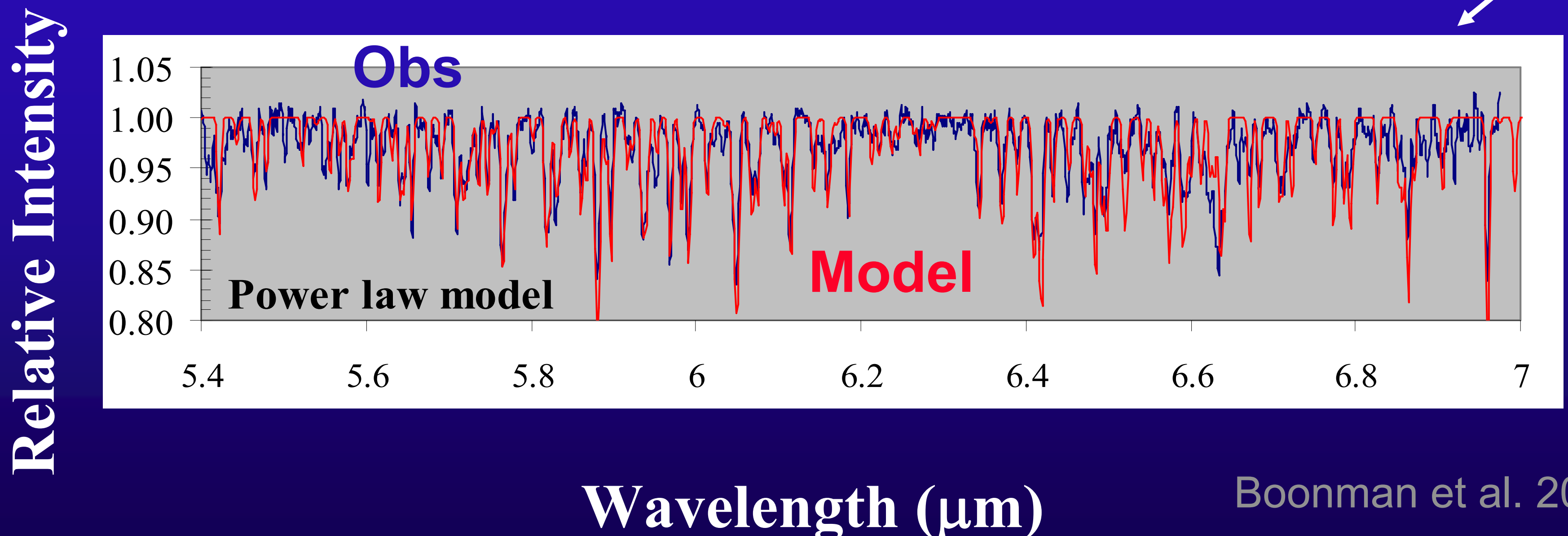
$x(H_2O) \sim 3 \times 10^{-6}$ ~ constant!



# *ISO-SWS – 6μm Absorption*

Significant (~10%) 6μm absorption detected
Constrains relative hot & cold water columns
Suggests both evaporation & depletion necessary

Results imply N($H_2O$) ~ 3 x $10^{18}$ $cm^{-2}$




Boonman et al. 2003

# *Our Question: Age & Evolution*

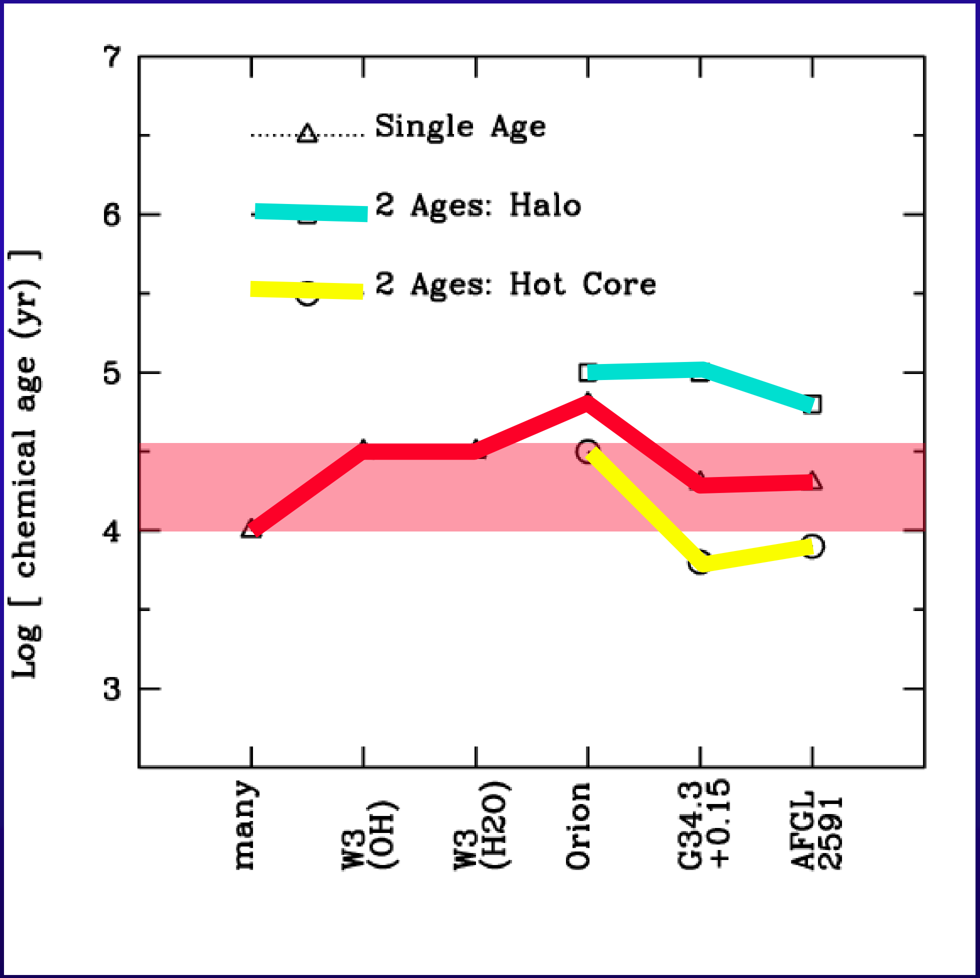
Evolution timescale of massive stars ~ $10^5$ yr [counting statistics]

Hot cores all seem to be same age! (~ $10^4$ yr)

Hot cores younger than surrounding envelopes

Why???

What does this imply for evolution?



# *Parcel Infall: Hot Gas Conditions*

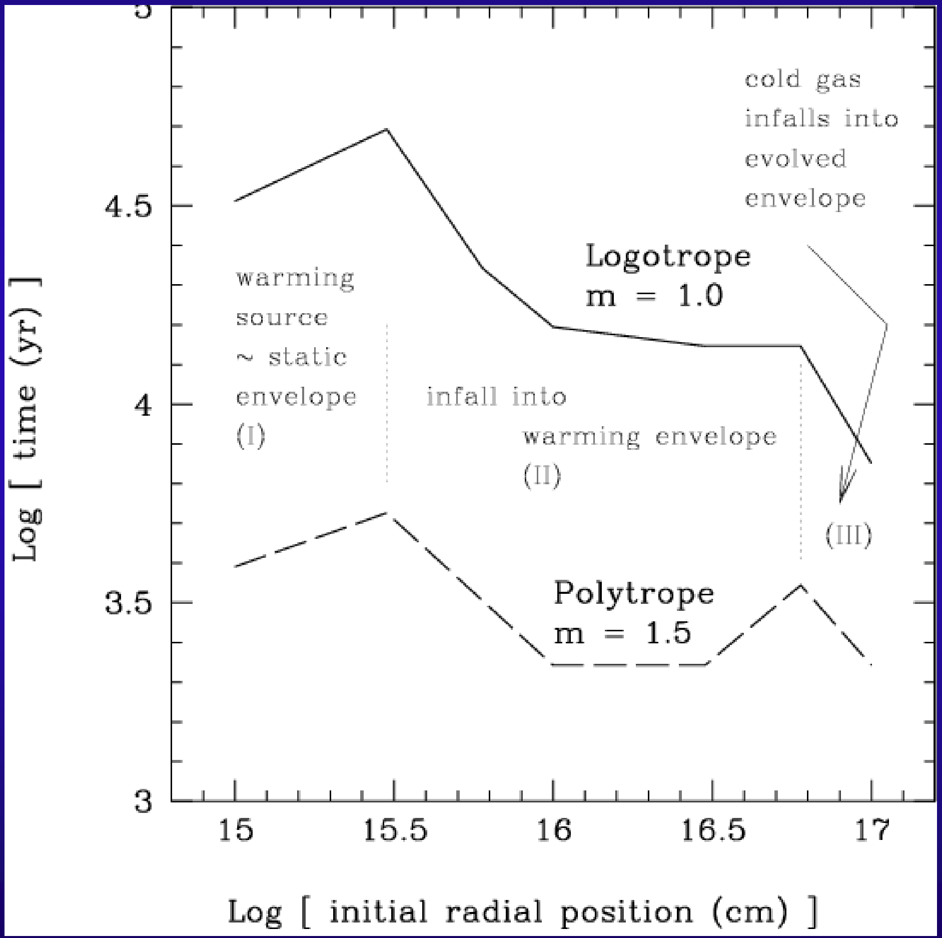
There exist 3 regimes for the hot gas

(I) warming, ~static

(II) infall into warming envelope

(III) cold gas falls into evolved env.

Hot gas lifetimes (>200AU) ~ $10^4$ yr +/- 0.5 dex



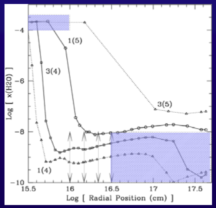

Naturally explains range of inferred ages

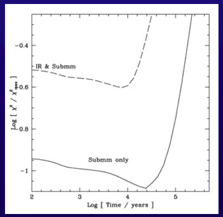
*Doty et al. 2006*

# *Implications for Age & Evolution*

It appears that we can successfully use chemistry in an infalling envelope modified by an evolving central YSO to age-date the (1) YSO, and (2) core + envelope

In AFGL 2591, the YSO appears to be ~ 3 – 10 x $10^4$ yr old.  The envelope (~ $10^5$ yr) is older than the hot core (~ $10^4$ yr).



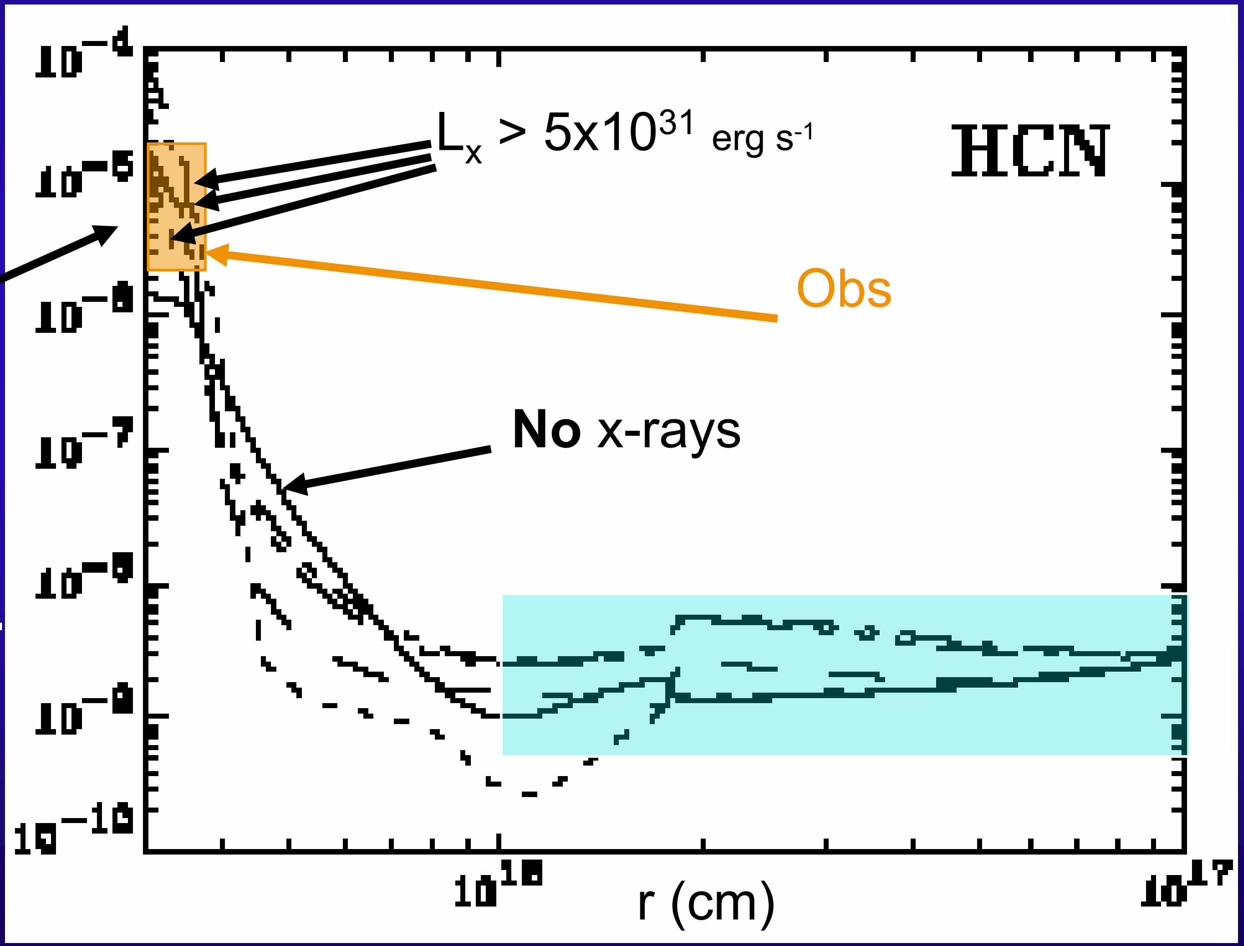
# *HCN: X-rays?*

Staeuber et al (*2005*) consider xray driven chemistry; improves chemical models

X-rays enhance HCN for r<4x10[15]

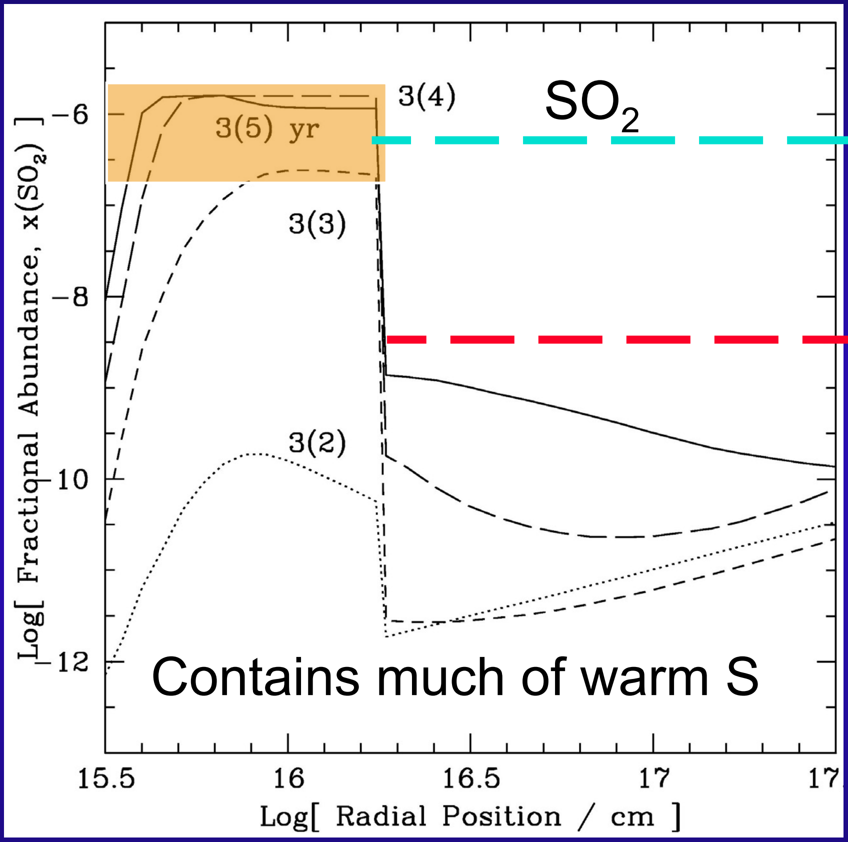
Consistent w/ obs.

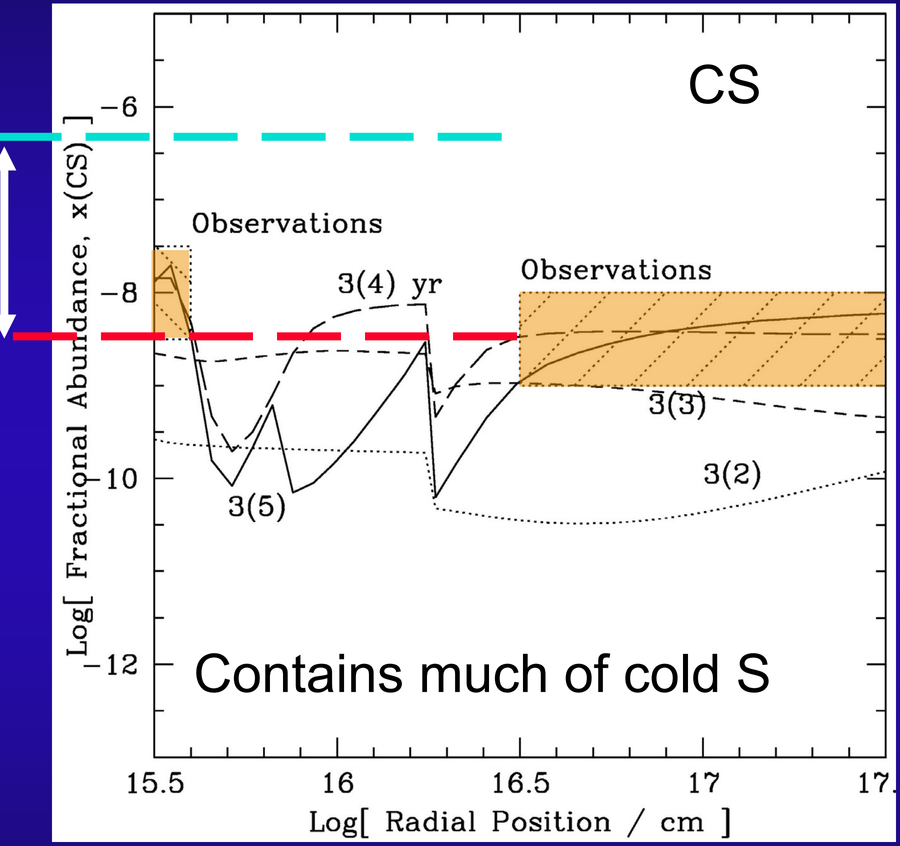
X-rays important?




Staeuber et al. 2005

# *Sulphur Abundance*




Extra warm gas-phase Sulphur:
Liberated from grains at 100K? Form for T < 100?

# *Explict Source Evolution*

- Envelope collapse *(infall from cool/sparse to warm/dense)*
- Stellar evolution $L_*(t)$ *[McKee & Tan 2003]* => $T(r,t)$
- Material ad/desorption