Tracing Pumping Routes in OH

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Understanding OH Pumping

- Analytic estimates backed by numerics[3 4] [1 5 2]
- Inferences from parameter-space searches
- Thermodynamic schemes[10]
- Monte-Carlo technique used on water masers[11]
- Analogy with currents + Monte-Carlo on methanol[12]
- How do we manage ‘complexity’?
- Problem not confined to maser studies

Elitzur et al.[3], Elitzur [4], Bujarrabal et al.[1], Sobolev [10], Elitzur [5], Dickinson [2], Sobolev [11], Sobolev & Deguchi[12]

Population Tracing

- RT solutions from numerical method (e.g. LU-factorization)
- Numerical results (level populations, mean intensities) are computed, but much physical insight lost
- The code TRACER restores population transfer information.
- A converged model is re-solved by the naive method
- Coefficient $k^z_{x,y}$ now has a simple interpretation:
- ...rate coefficient for transfer of population from level x to level y with z eliminations to go.

An Example

- Choose $x = 2$, $y = 10$ and $z = 16$.
- Look at modification to next elimination, $z = 15$.
- $k^{15}_{2,10} = k^{16}_{2,10} + k^{16}_{2,15} k^{16}_{15,10} / k^{16}_{15,15}$
- Begin at small value of z and work back
- Eventually expand to coefficients with $z = N + 1$: N is the number of energy levels in model.
- No guarantee of simplicity!

Additional Detail

- Start from a small matrix (e.g. 3×3).
- Solve for inversion in required line.
- Organise rate-coefficents: antagonistic pairs
- ‘Direct’ and ‘Indirect’ parts of pump
- Begin computer analysis with TRACER
- Reduce all rate coefficients to unmodified form.

The 1612 MHz Inversion

- The formula for the 1612 MHz inversion, at $z = 4$ is
-

$$\Delta\rho_{32} = \frac{\mathcal{N} k_{1,2}^4}{D}\left\{(1+\eta)\left(\frac{k_{2,3}^4}{3} - \frac{k_{3,2}^4}{5}\right) + \frac{\eta k_{2,1}^4}{3} - \frac{k_{3,1}^4}{5}\right\}$$

- ...where $\eta = k_{1,3}^4 / k_{1,2}^4$
- First part is ‘direct pump’
- Second part gives ‘indirect’ pump via level 1:

Other Ground-State Inversions

$$\Delta\rho_{31} = \frac{\mathcal{N} k^4_{2,2}}{3D}\left\{k^4_{1,3} - k^4_{3,1} + \left(\frac{k^4_{1,2}k^4_{2,3} - k^4_{3,2}k^4_{2,1}}{k^4_{2,2}}\right)\right\}$$

$$\begin{aligned}\Delta\rho_{42} \;=\; \frac{\mathcal{N}'}{5}\Bigg\{ & k^5_{2,4} - k^5_{4,2} + \frac{k^5_{1,1}}{X}(k^5_{2,3}k^5_{3,4} - k^5_{4,3}k^5_{3,2}) + \frac{k^5_{3,3}}{X}(k^5_{2,1}k^5_{1,4} - k^5_{4,1}k^5_{1,2}) \\ & + \frac{k^5_{2,1}k^5_{1,3}k^5_{3,4} - k^5_{4,3}k^5_{3,1}k^5_{1,2}}{X} + \frac{k^5_{2,3}k^5_{3,1}k^5_{1,4} - k^5_{4,1}k^5_{1,3}k^5_{3,2}}{X}\Bigg\}\end{aligned}$$

$$\begin{aligned}\Delta\rho_{41} \;=\; \mathcal{N}'\Bigg\{ & \frac{k^5_{1,4}}{5} - \frac{k^5_{4,1}}{3} + \frac{k^5_{3,3}}{X}\left(\frac{k^5_{1,2}k^5_{2,4}}{5} - \frac{k^5_{4,2}k^5_{2,1}}{3}\right) + \frac{k^5_{2,2}}{X}\left(\frac{k^5_{1,3}k^5_{3,4}}{5} - \frac{k^5_{4,3}k^5_{3,1}}{3}\right) \\ & + \frac{k^5_{1,2}k^5_{2,3}k^5_{3,4}}{5X} - \frac{k^5_{4,3}k^5_{3,2}k^5_{2,1}}{3X} + \frac{k^5_{1,3}k^5_{3,2}k^5_{2,4}}{5X} - \frac{k^5_{4,2}k^5_{2,3}k^5_{3,1}}{3X}\Bigg\}\end{aligned}$$

Example Pump Traces

- 1612 MHz in a deteched Mira envelope - study of envelope detachment; time dependence
- 1612 and 1667 MHz in a larger envelope (M-type supergiant); 35 micron lines
- 1665 MHz for typical star-forming region
- 1667 MHz (conditions as for 1665)

1612 MHz Inversion

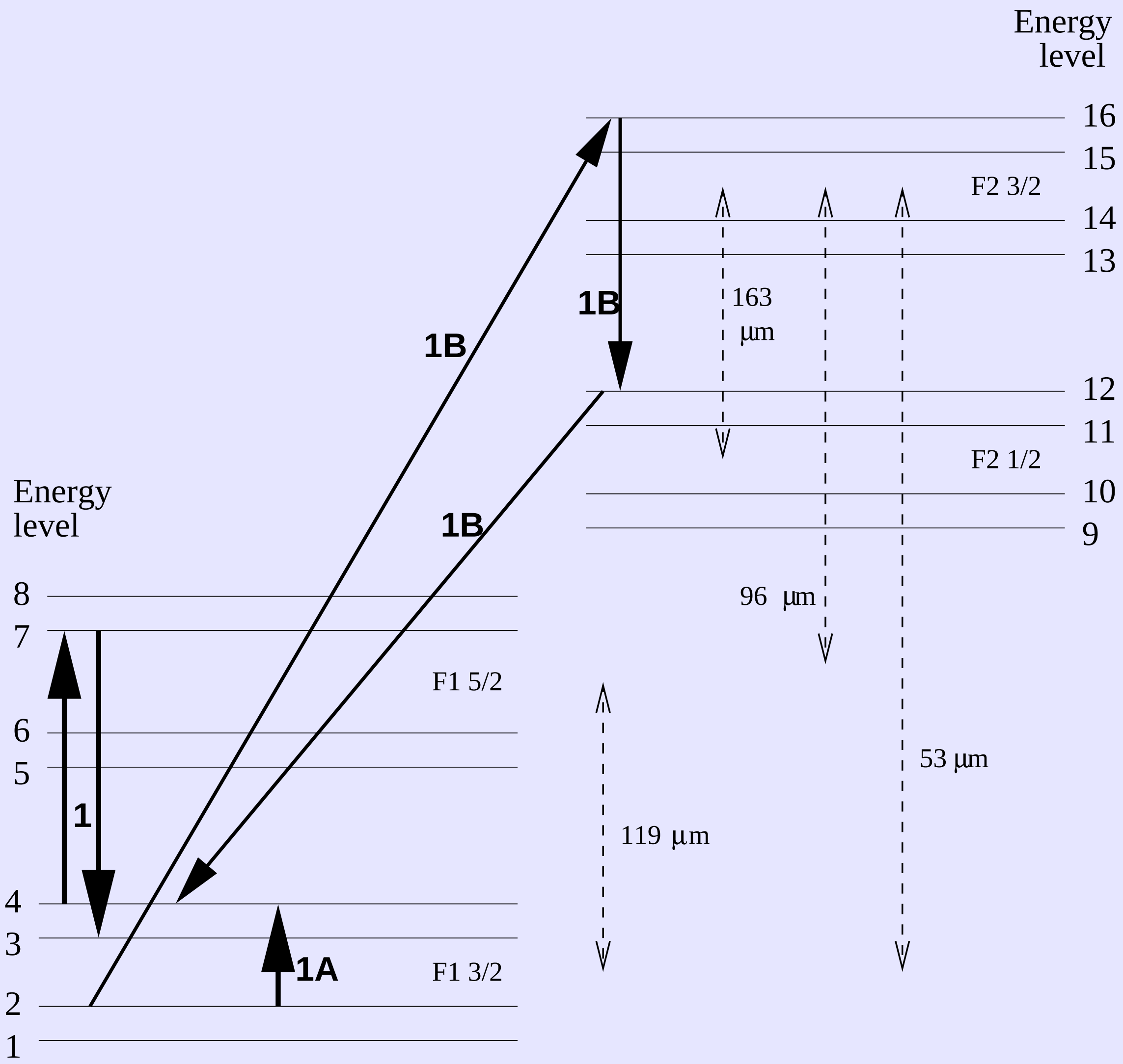
- Formula for indirect pump:

$$\frac{1}{k_{1,2}^{4}}\left[\left(\frac{k_{2,1}^{4}}{3}\right)k_{1,3}^{4} - k_{3,1}^{4}\left(\frac{k_{1,2}^{4}}{5}\right)\right]$$

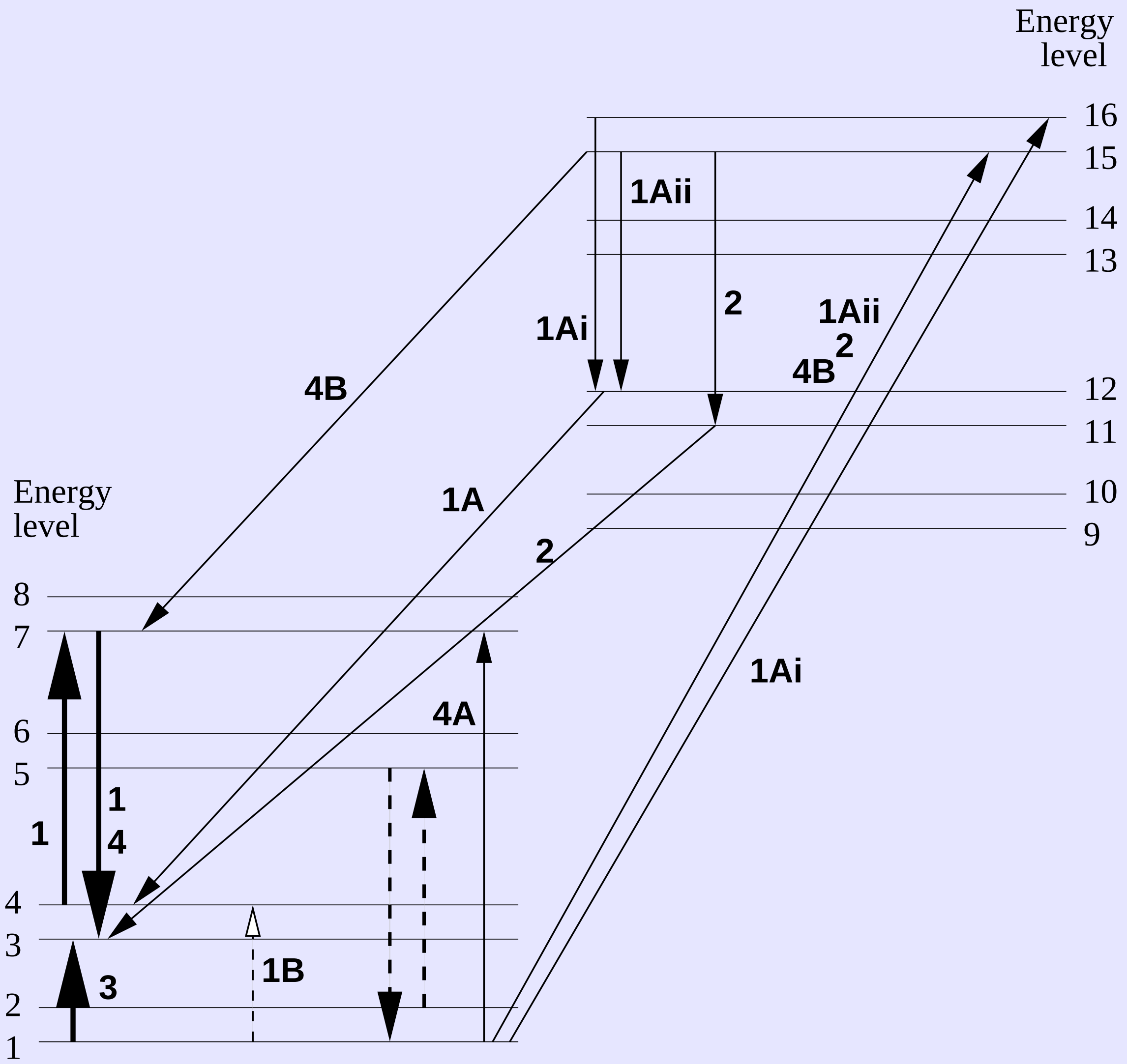
- At shell detachment, 2/3 of pump is ‘direct’
- Most of loss of gain 40 yr later due to collapse of *indirect* pump.
- Publication of results (2005)[7]

Gray et al.[7]

Diagram: Routes of the Direct Pump



Routes for the Indirect Pump



Summary

- Most important radiative pump uses 53 μm radiation.
- Routes via level 1 more dependent on 53 μm photons.
- Expanding detached shell cools.
- 53 μm energy density reduces with time.
- Vulnerable part of pump (via level 1) collapses
- 1612 MHz line in absorption $\sim$ 50 yr after detachment.

1612/65 MHz: Larger Envelope

- Model of M supergiant
- 35 micron radiation important
- model based on S Per (M4.5)
- 1612 MHz pump more like traditional scheme[3]
- 1665 MHz pump (shown) returns without $^2\Pi_{1/2}, J = 1/2$ to $^2\Pi_{3/2}, J = 3/2$
- strongest routes in black (then green, purple)

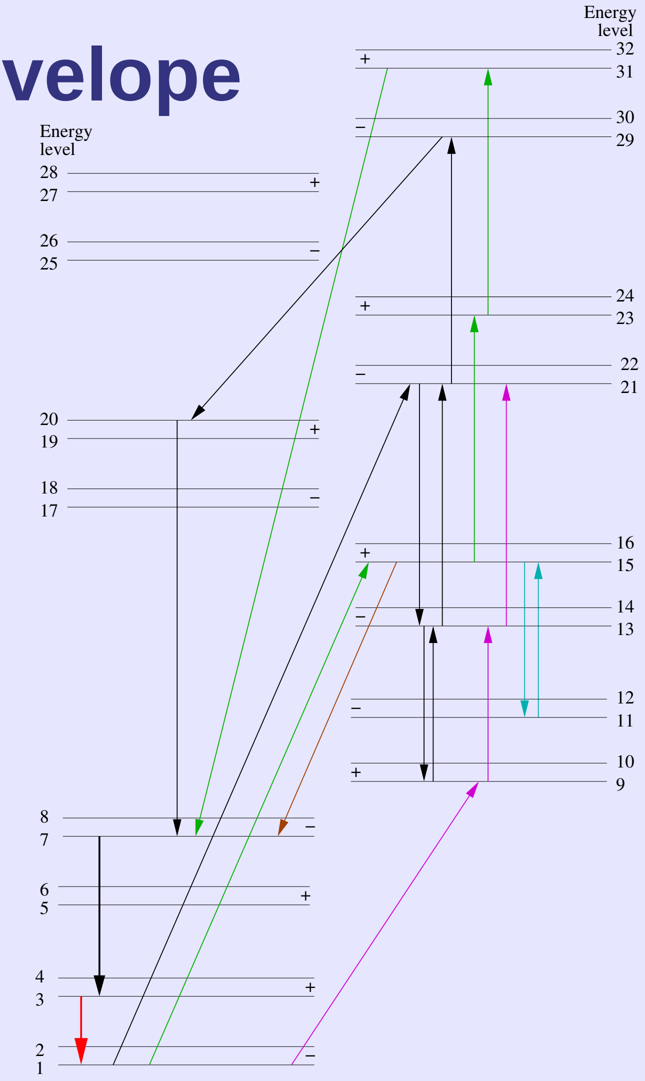


Figure 1: Pump routes for 1665 MHz in an M-supergiant

Elitzur et al.[3]

Star-Forming Regions

- Model: part of parameter-space search
- Slab ALI solution with strong main-line inversions:
- 48 levels, conditions as follows:
    - 80 log-spaced depths in 2×10^{13} m
    - n$_{H_2}$ = 10^7 cm^{-3}; [OH] = 0.2 ppm
    - T$_K$ = 30 K; T$_d$ = 70 K
    - no microturbulence; no velocity gradient
    - unsaturated integrated gains: 20.039 at 1665 MHz; 35.661 at 1667 MHz

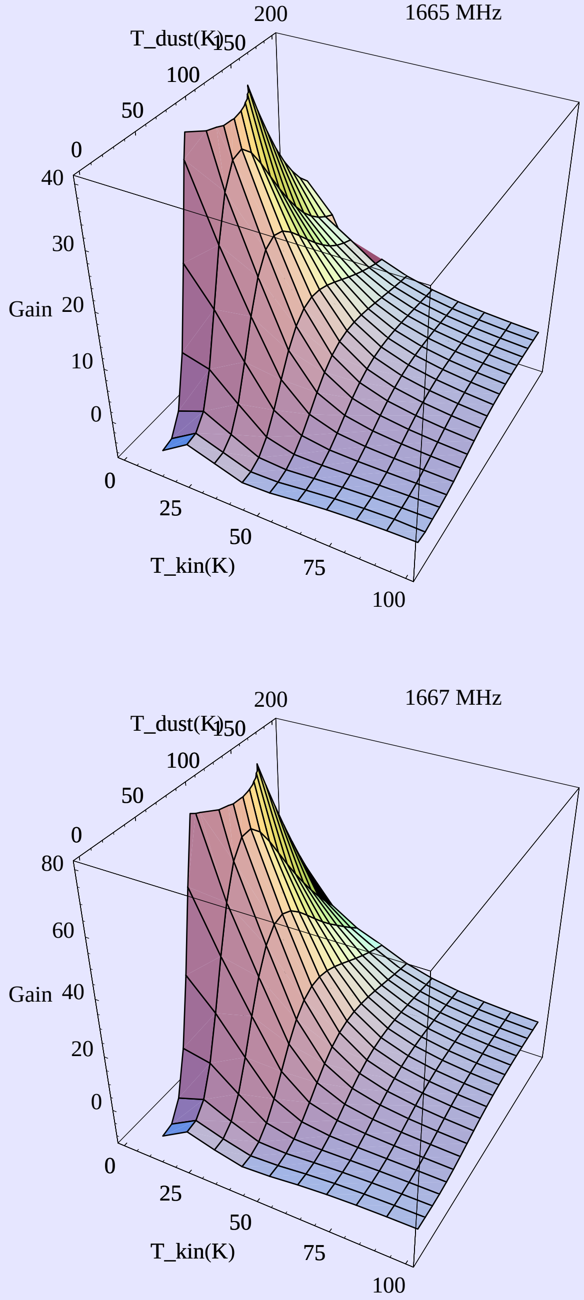


Figure 2: Parameter-space plots: 1665 & 1667 MHz

1665 MHz Trace

- (i) $k^{4}_{1,3} - k^{4}_{3,1} = 1.05\times 10^{-4}\,s^{-1}$
- (ii) $(k^{4}_{1,2}k^{4}_{2,3} - k^{4}_{3,2}k^{4}_{2,1})/k^{4}_{2,2} = 9.07\times 10^{-5}\,s^{-1}$
- Two dominant routes in (i) supply 83% of it.
- Three dominant routes in (ii) supply 80.5% of it.
- These break down to a set providing 82% of the total:
  - (i) $(k^{6}_{1,5}k^{6}_{5,3} - k^{6}_{3,5}k^{6}_{5,1})/k^{6}_{5,5} = 6.01\times 10^{-5}\,s^{-1}$
  - (ii) $(k^{6}_{1,5}k^{6}_{5,2}k^{6}_{2,4}k^{6}_{4,3} - k^{6}_{3,4}k^{6}_{4,2}k^{6}_{2,5}k^{6}_{5,1})/(k^{4}_{2,2}k^{5}_{4,4}k^{6}_{5,5}) = 4.86\times 10^{-5}\,s^{-1}$
  - (iii) $(k^{5}_{1,4}k^{5}_{4,3} - k^{5}_{3,4}k^{5}_{4,1})/k^{5}_{4,4} = 2.72\times 10^{-5}\,s^{-1}$
  - (iv) two further terms totalling $2.46\times 10^{-5}\,s^{-1}$

Further Complexity

- Route (i) has no additional complexity!
- Route(ii) very complex but 3 routes control 73% of it:
  (A) a route via levels 4, 6 and 7;
  (B) a route via level 20 (in F1, J=7/2);
  (C) via levels 10 and 14 (visits F2, J=1/2 & 3/2)
- Route (iii) is worse still: top 3 routes comprise 50%:
  (A) web of routes via 9, 10, 14 and 20;
  (B) a route via 10 and 14, excluding level 9;
  (C) a route involving a collisional transfer from 4$\rightarrow$ 3

1665 MHz Pump

- the most important route
- energy levels not to scale
- pump entirely in F1
- upward step radiative
- downward step collisional
- reverse routes not shown

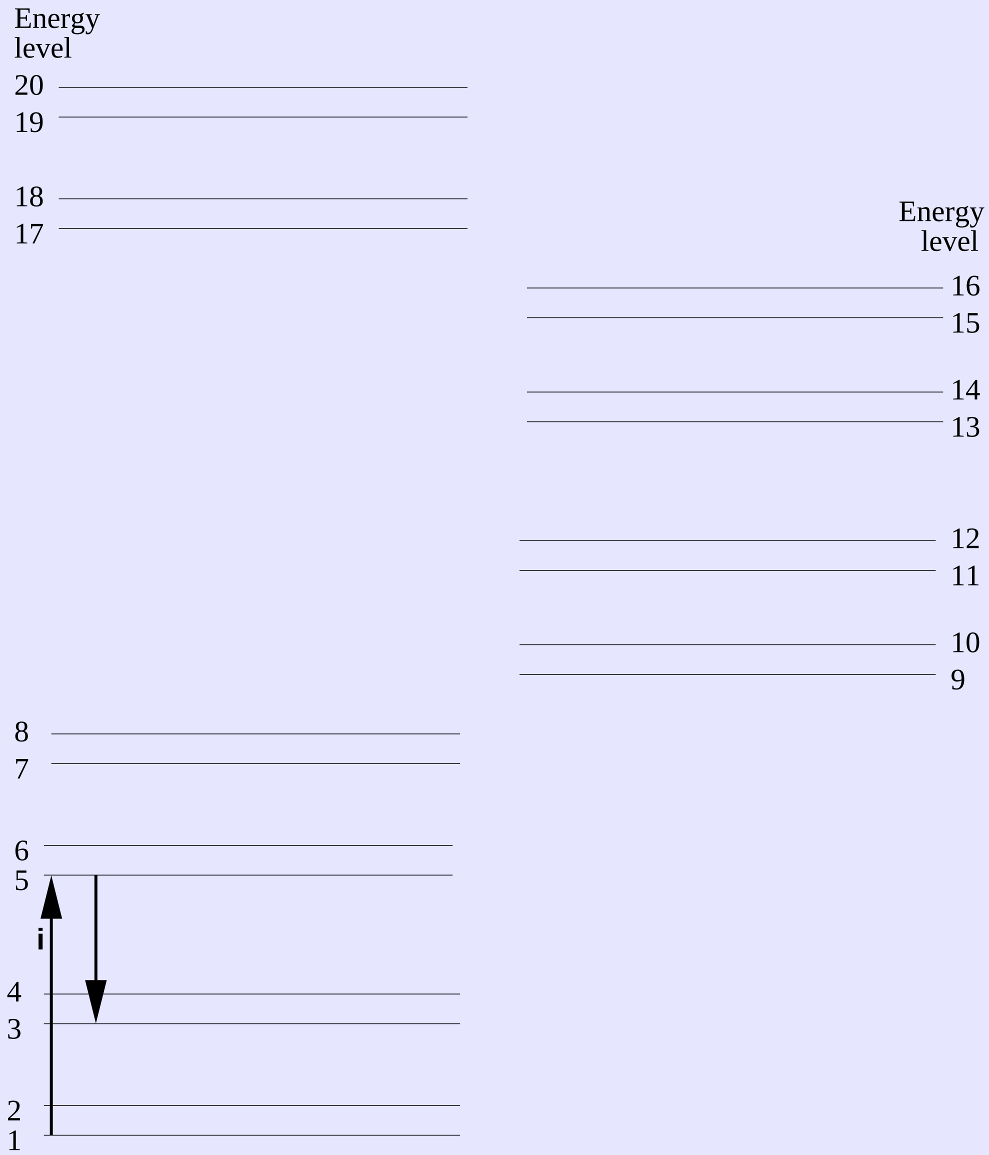


Figure 3: Strongest Pump Routes at 1665 MHz

1665 MHz Pump

- the two most important routes
- energy levels not to scale
- pump predominantly in F1
- mostly radiative steps
- some collisional steps, e.g. 5⟶ 3 and 6⟶ 4
- upward routes only shown

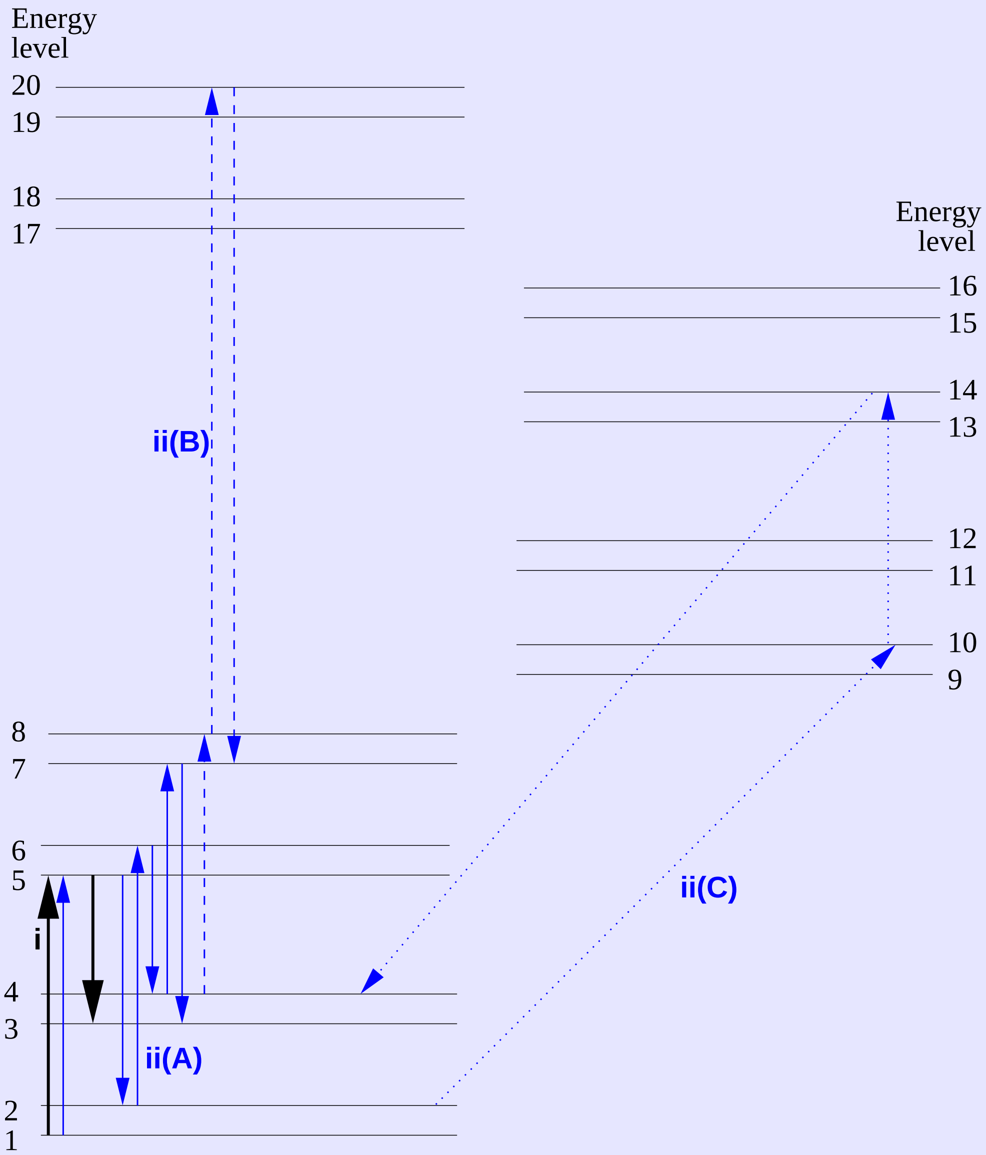


Figure 4: Strongest Pump Routes at 1665 MHz

1665 MHz Pump

- 3 most important routes
- energy levels not to scale
- pump predominantly in F1 BUT
- route iii uses F2 stack a lot
- mostly radiative
- several important collisional links
- upward routes only shown

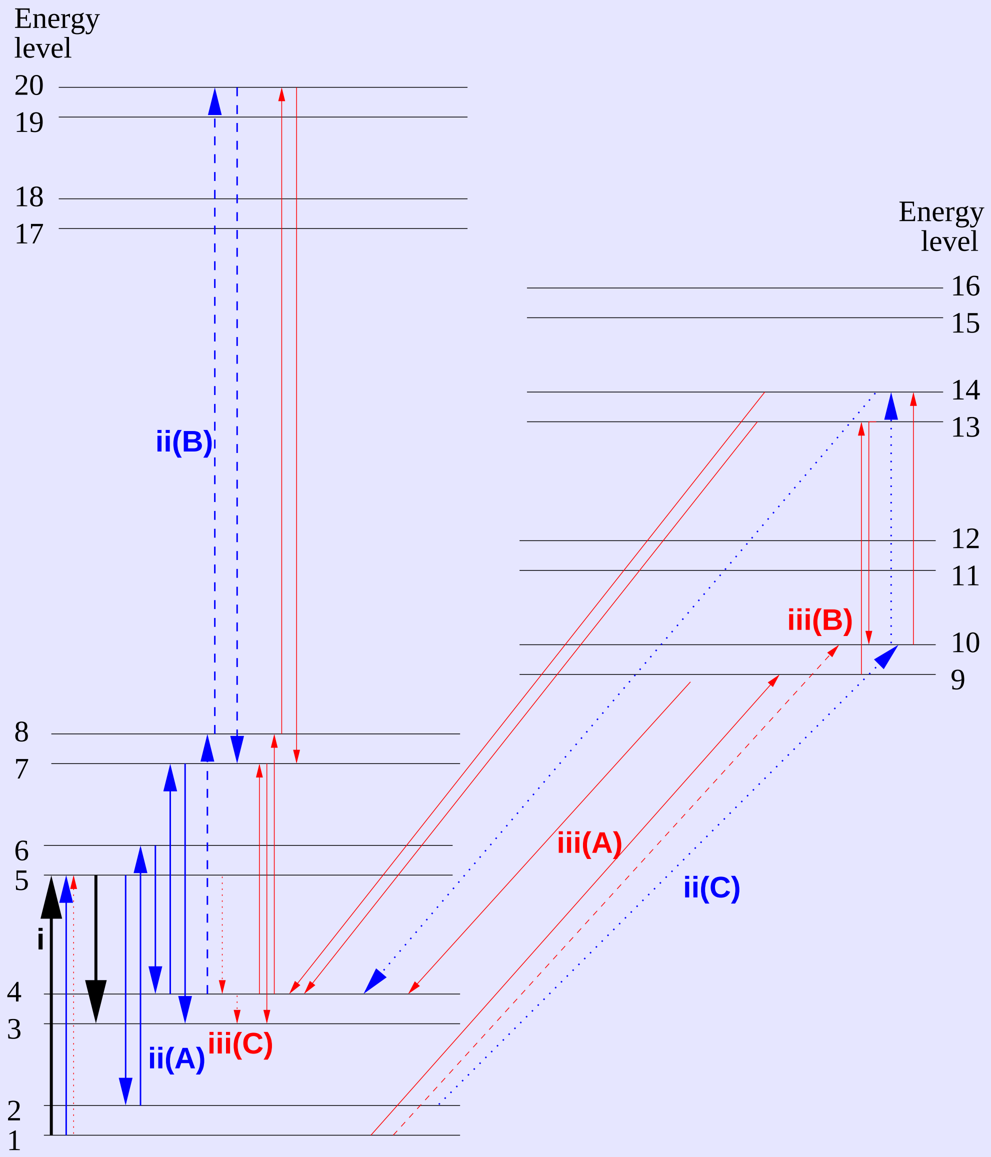


Figure 5: Strongest Pump Routes at 1665 MHz

1667 MHz Pump

- relative strengths:
- i = 1.0
- ii = 0.413
- iii = 0.290
- iv = 0.255
- v = 0.228
- vi = 0.203
- vii = 0.112

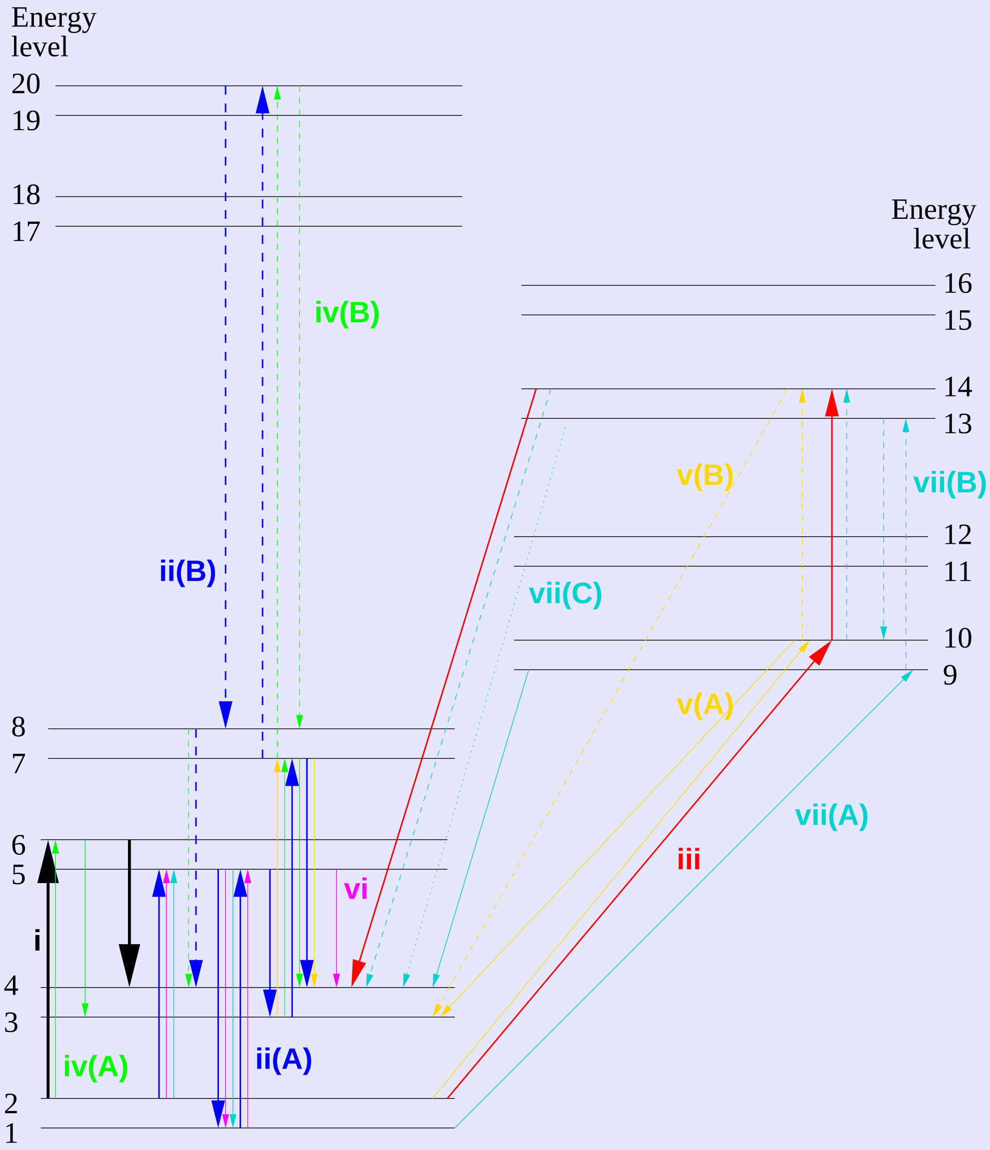


Figure 6: Strongest Pump Routes at 1667 MHz

1665 and 1667 Compared

- Detailed results now published [6]
- Pumps share many features.
- Routes in F1 stack are dominant
- Strongest route goes only to F1, J=5/2
- 1 → 5 + 5 → 3 in 1665; 2 → 6 + 6 → 4 in 1667
- radiative ‘up’; collisional ‘down’
- Weaker routes use F2 stack much more.

Gray [6]

At a Deeper Level

- Expand rate coefficients: radiative & collisional parts
- Example: strongest 1665 MHz pump
- $k_{1,5}k_{5,3} - k_{3,5}k_{5,1}$ expands as:

$$[B_{1,5}\bar{J}_{1,5} + C_{1,5}]C_{5,3} - C_{3,5}[A_{5,1} + B_{5,1}\bar{J}_{1,5} + C_{5,1}]$$

- Values in Hz: $C_{5,3} = 3.75(-4); C_{3,5} = 1.13(-5)$
  $A_{5,1} = 0.1244; B_{5,1}\bar{J}_{1,5} = 2.160(-2); C_{5,1} = 3.16(-4)$
  $B_{1,5}\bar{J}_{1,5} = 3.60(-2); C_{1,5} = 9.48(-5)$
- Ignore cross-products of collision terms

What is Responsible?

- Also, $C_{5,3} \gg C_{3,5}$ (by a factor > 10) so,
- $k_{1,5}k_{5,3} - k_{3,5}k_{5,1} \sim B_{1,5}\bar{J}_{1,5}C_{5,3} - A_{5,1}C_{3,5}$
- Put Bs and Cs in terms of downward coefficients

$$k_{1,5}k_{5,3} - k_{3,5}k_{5,1} \sim (C_{5,3}g_5/g_1)[B_{5,1}\bar{J}_{1,5} - A_{5,1}e^{-\frac{h\nu}{kT_K}}]$$

$$= \frac{A_{5,1}C_{5,3}g_5/g_1}{e^{-\frac{h\nu}{kT_K}}}\left[\frac{\bar{J}_{1,5}}{B_\nu(T_K)} - 1 + e^{-\frac{h\nu}{kT_K}}\right]$$

- The exponential is $\ll 1$

The Answer?

- Multiplier is just a rate: says nothing about inversion
- $k_{1,5}k_{5,3} - k_{3,5}k_{5,1} \sim K((\bar{J}_{1,5}/B_\nu(T_K) - 1)$
- Inversion depends on two things:
- (i) 3→5 energy gap large for T_K
  - favours $C_{5,3}$ over $C_{3,5}$.
- (ii) Dust continuum (at $T_d = 70\,$K) hotter than T_K
  - allows mean intensity $>$ black-body at T_K.

Digging Deeper Still

- Source of 70 K radiation is optically thick boundary
- Radiation diffusion approximation applicable here
- $\frac{\bar{J}_{1,5}}{B_\nu(T_K)} - 1 = \left[\frac{B_\nu(T_d)}{B_\nu(T_K)} - 1\right] e^{-\sqrt{3\zeta}(\tau_M - \tau)}$
- scattering parameter ζ modifies optical depth
- value $\zeta \sim C_{5,1}/A_{5,1} = 3.51(-4)$
- Radiation is not thermalised

Parity Propensity

- Why do ‘mirror routes’ not cancel inverting effects?
- Example: route linking levels 3 and 1 via 7 (instead of 5)
- $C_{7,1}$ is considerably smaller than $C_{5,3}$
- $C_{7,1}$ not leading term in TRACER expansion
- Contribution from collisions with para-hydrogen is explanation
- Parity propensity disappears at temperatures above 100 K
- no propensity in OH + ortho-H_2

Future Plans

- Additional scenarios: SNR 1720 MHz; megamasers
- How typical are these pumps?
- Increase automation
- Role of velocity gradients
- Extend method to other molecules: H_2O in progress
- Extend method to excited states
- Other problems reducible to pseudo-linear algebra

Conclusions

- Expanding all-process rate-coefficients can reveal pump routes
- Routes can be separated into inverting and anti-inverting sets.
- For ‘dying’ OH-IR stars decay of gain is mainly caused by changes to the routes operating via level 1
- Larger, ‘supergiant’, envelopes rely more on 35 micron radiation
- In star-forming regions, main-line pump is mainly radiative but with crucial collisional steps.

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