A NEW METHODOLOGY FOR THE DETECTION OF LOW-ABUNDANCE SPECIES IN THE ISM

DETECTION OF INTERSTELLAR CARBODIIMIDE (HNCNH)

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Geoffrey A. Blake • Jan M. Hollis • Frank J. Lovas • Philip R. Jewell • Anthony J. Remijan

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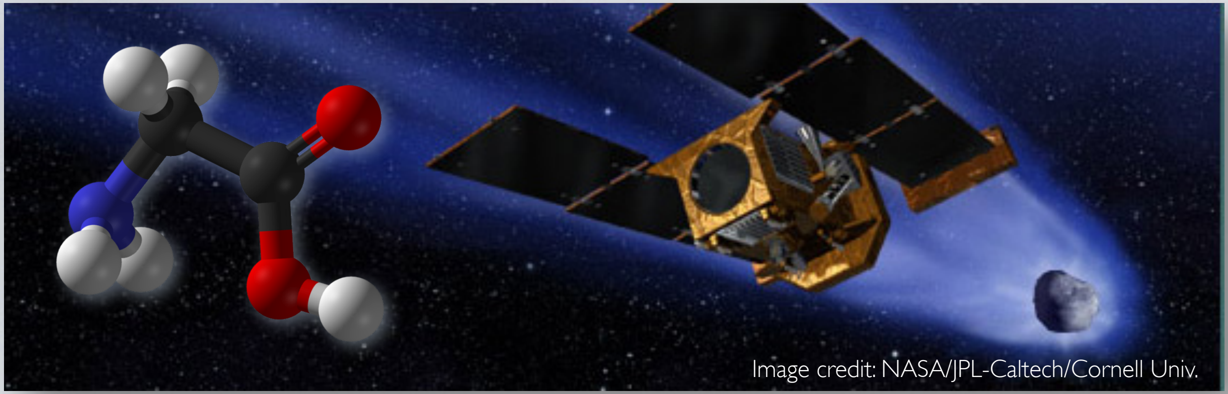
INTRODUCTION



Elsila et al., 2009, Meteor. Planet. Sci., 44, 1323
Garrod, R.T., 2013, ApJ, 765, 60

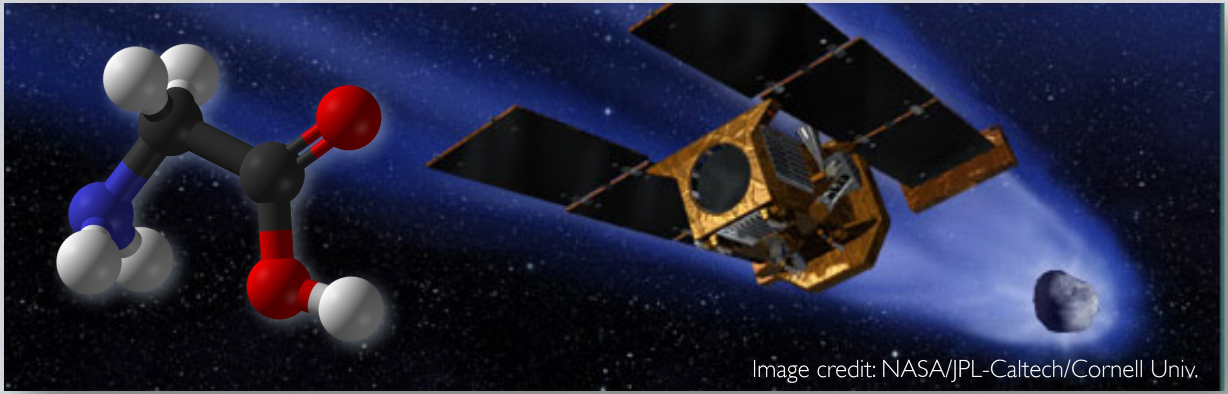


Image credit: NASA/JPL-Caltech/Cornell Univ.

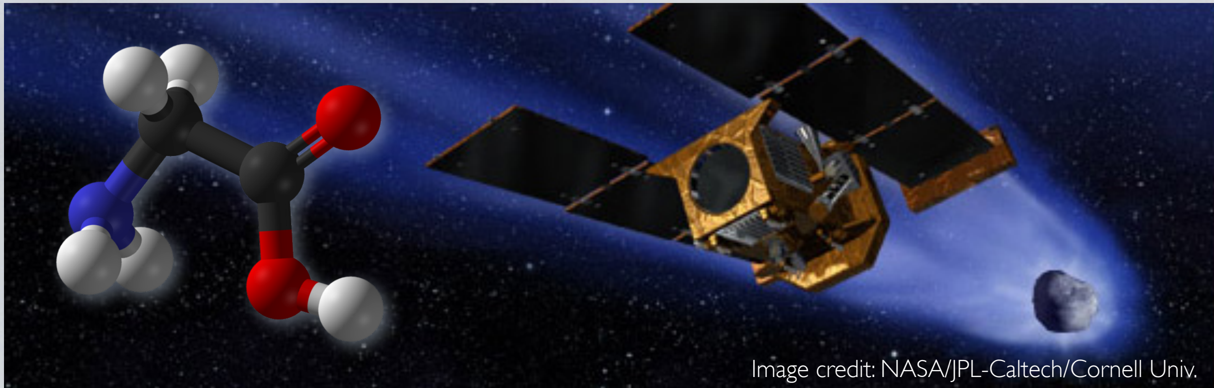
Where?

When?

How?

Elsila et al., 2009, Meteor. Planet. Sci., 44, 1323
Garrod, R.T., 2013, ApJ, 765, 60

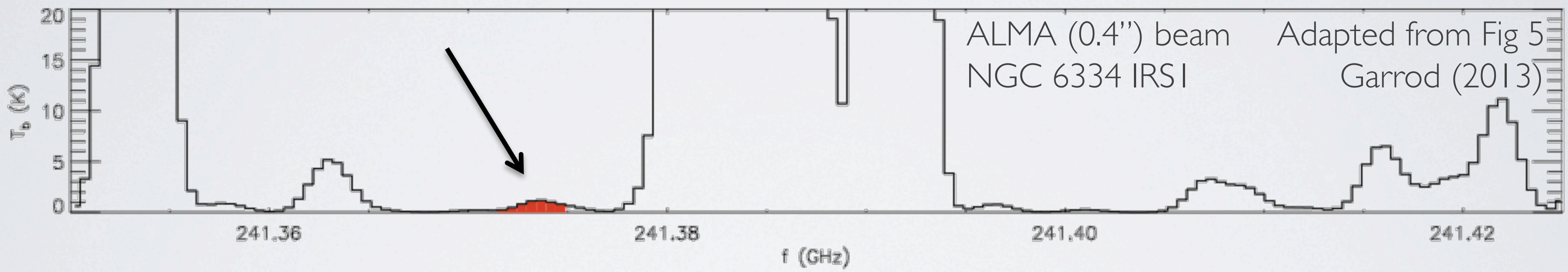
INTRODUCTION



Where?

When?

How?



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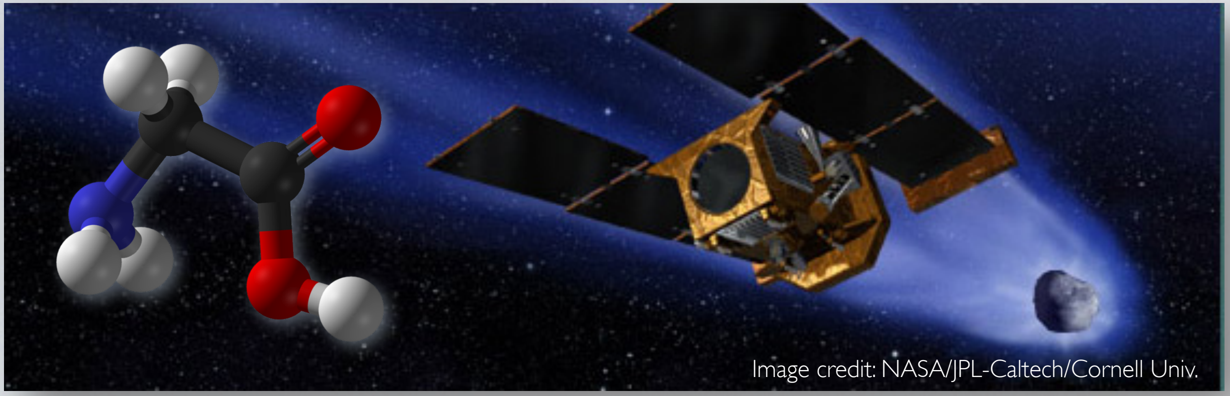
INTRODUCTION



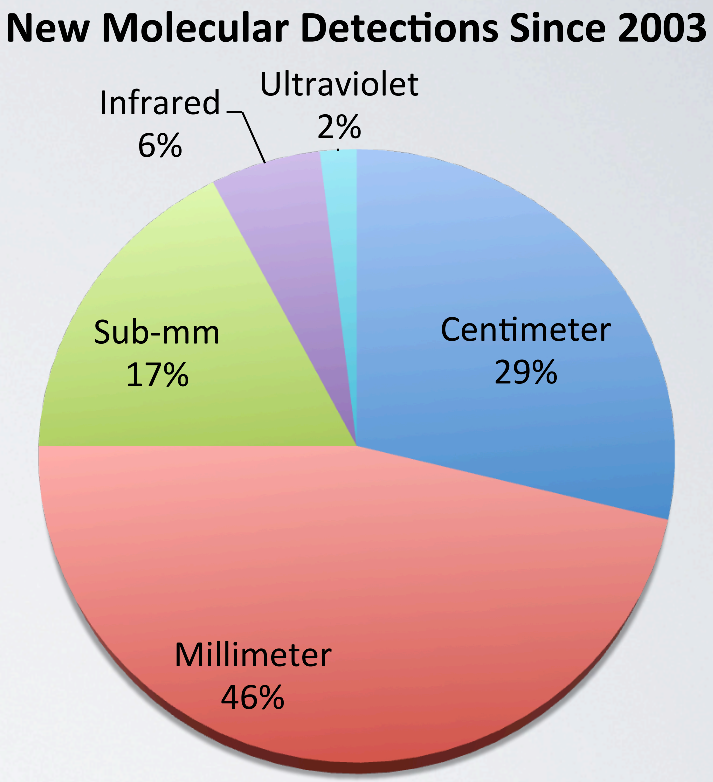
Where?

When?

How?

Better Chemical Inventories yield better predictions

Elsila et al., 2009, Meteor. Planet. Sci., 44, 1323
Garrod, R.T., 2013, ApJ, 765, 60

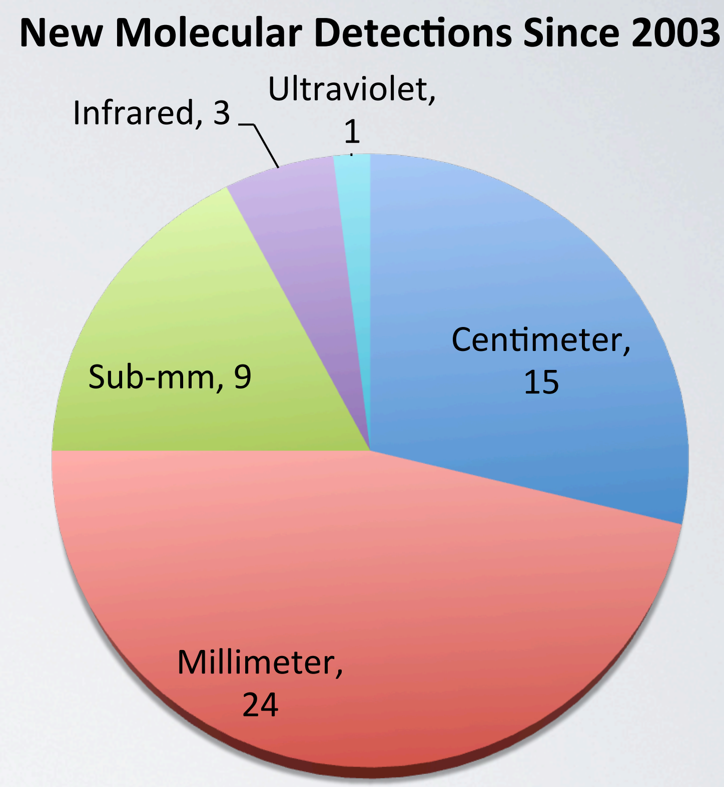

New Molecular Detections Since 2003
Infrared 6%
Ultraviolet 2%
Sub-mm 17%
Centimeter 29%
Millimeter 46%

Millimeter/sub-mm/THz

- Boltzmann peak of many COMs
- ALMA

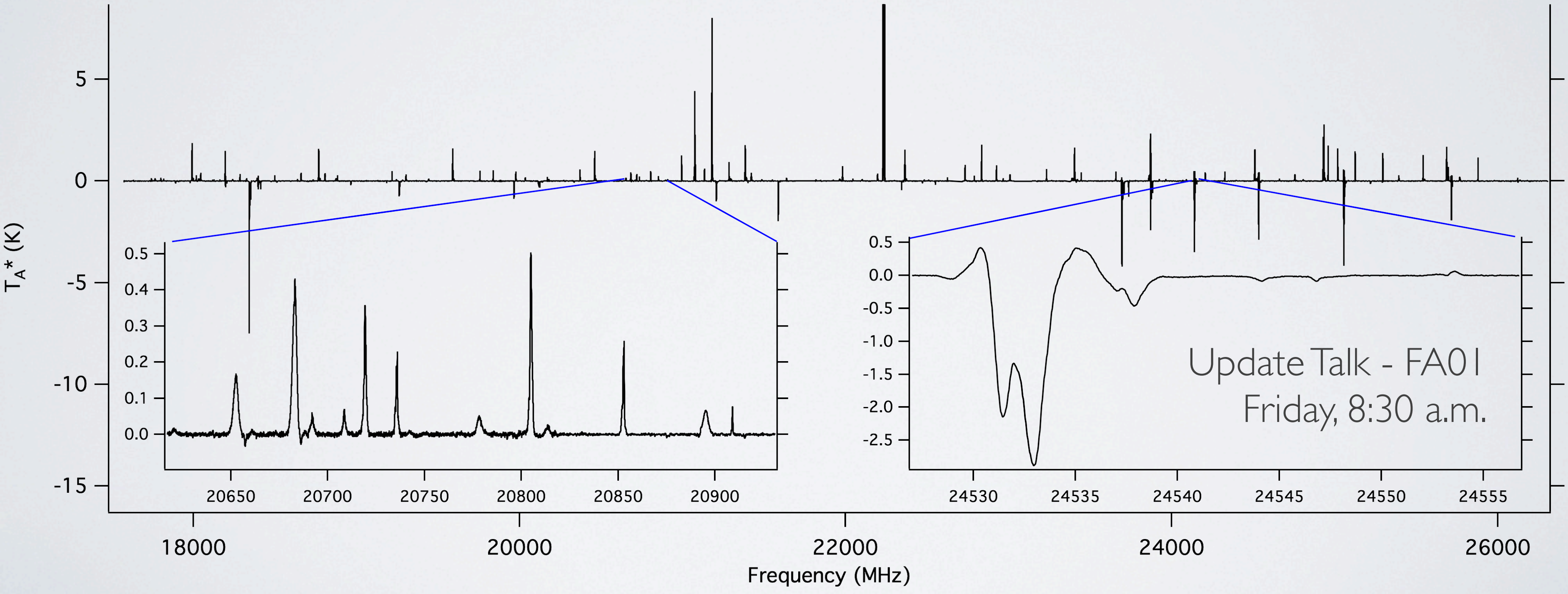
Centimeter

- Generally weaker transitions (LTE)
- Much lower line-density
- Rapidly achieve low RMS noise



PRebiotic Interstellar MOlecular Survey

- Targets Sgr B2(N) Complex
- Nearly continuous frequency coverage ~300 MHz - 50 GHz
- RMS of 2 - 10 mK
- Publicly available: www.cv.nrao.edu/~aremijan/PRIMOS



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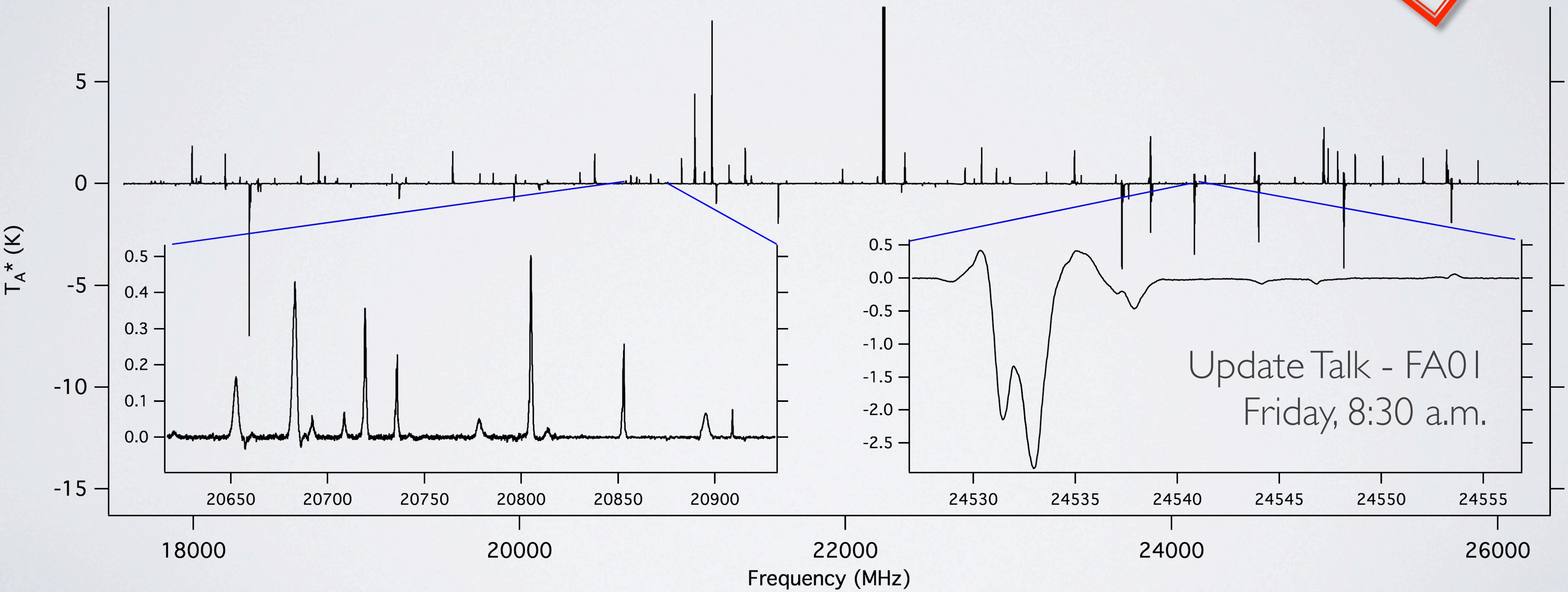
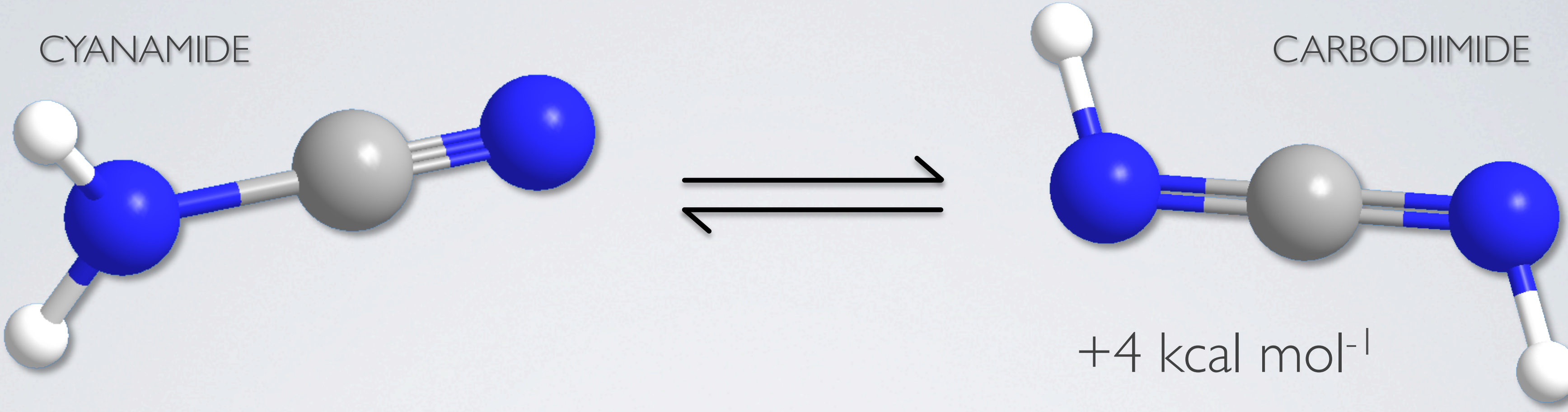
- Targets Sgr B2(N) Complex
- Nearly continuous frequency coverage ~300 MHz - 50 GHz
- RMS of 2 - 10 mK
- Publicly available: www.cv.nrao.edu/~aremijan/PRIMOS

No Proprietary Period



Update Talk - FA01
Friday, 8:30 a.m.

CARBODIIMIDE - CHEMISTRY

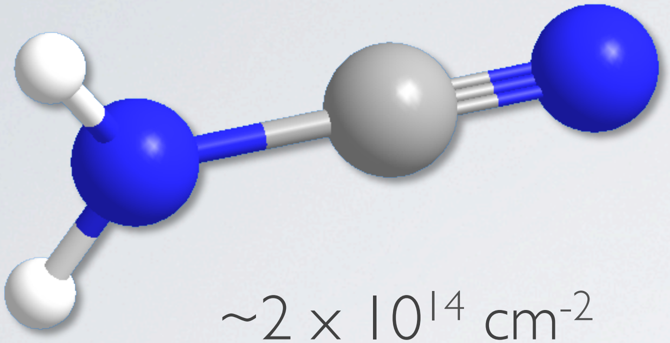


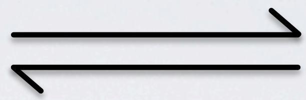
+4 kcal mol^{-1}

~1% at 300 K

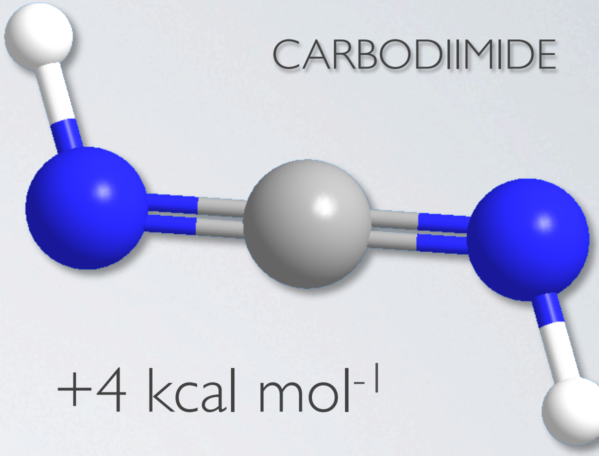
Nummelin et al., 2000, ApJS, 128, 213
Turner et al., 1975, ApJ, 201, L149

CYANAMIDE





CARBODIIMIDE

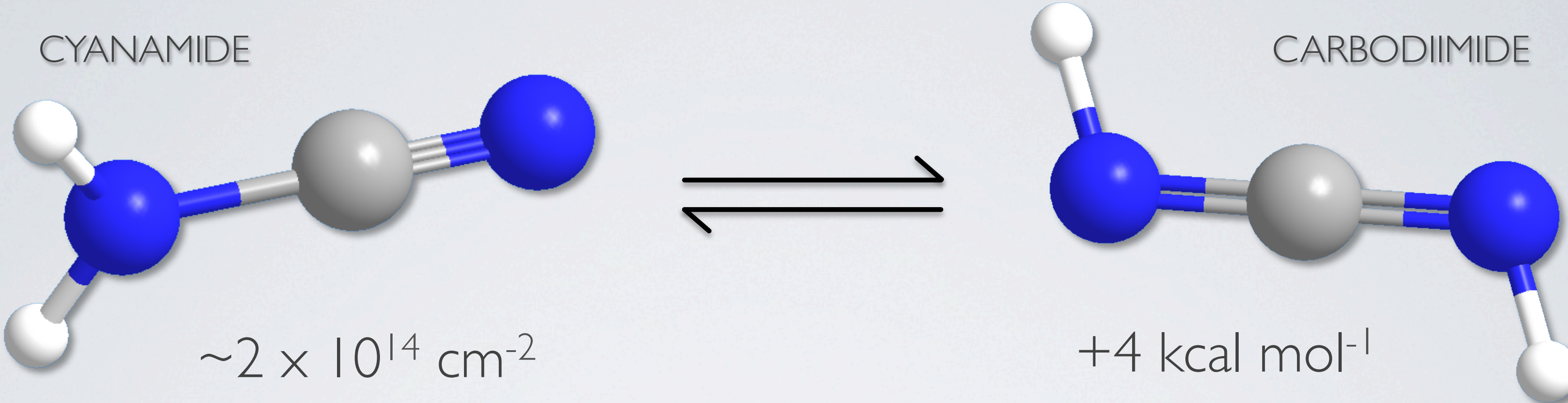


~2 x 10^{14} cm^{-2}
Sgr B2(N)

+4 kcal mol^{-1}
~1% at 300 K

- NH_2CN detected in 1975 (Turner et al.)
- HNCNH discounted due to low assumed abundance

Nummelin et al., 2000, ApJS, 128, 213
Turner et al., 1975, ApJ, 201, L149



~2 x 10^{14} cm^{-2}
Sgr B2(N)

+4 kcal mol^{-1}
~1% at 300 K

- NH_2CN detected in 1975 (Turner et al.)
- HNCNH discounted due to low assumed abundance

- Duvernay et al. (2005): conversion in water ice much more efficient

Nummelin et al., 2000, ApJS, 128, 213
Turner et al., 1975, ApJ, 201, L149

HNCNH Transitions

$18_{0,18} - 17_{1,17}$ { 4.3 GHz, 4.8 GHz

$19_{0,19} - 18_{1,18}$ { 25.1 GHz, 25.5 GHz

$20_{0,20} - 19_{1,19}$ { 45.8 GHz, 46.3 GHz

$16_{1,16} - 17_{0,17}$ { 15.9 GHz, 16.4 GHz

$15_{1,15} - 16_{0,16}$ { 36.7 GHz, 37.1 GHz

Torsional Doublets

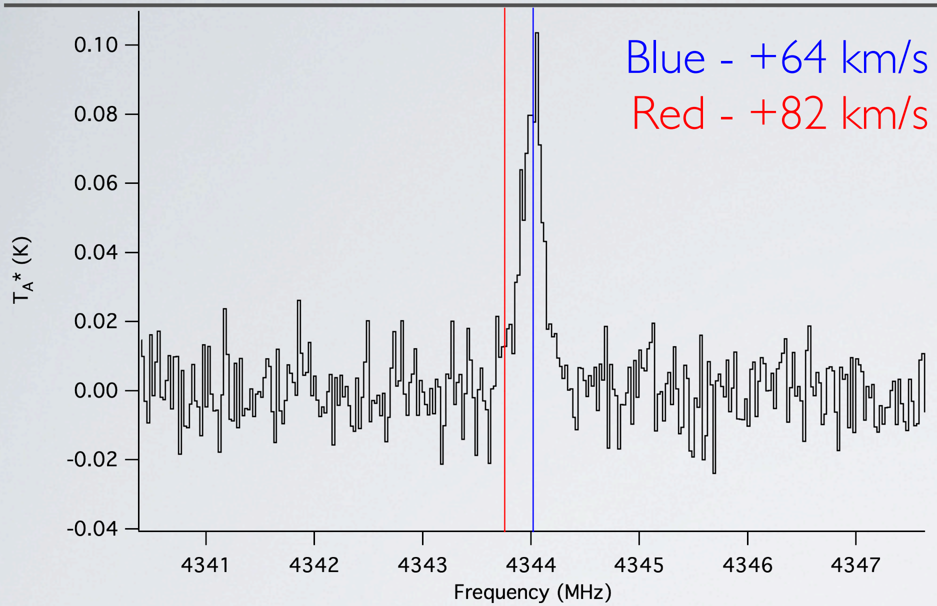
HNCNH Transitions

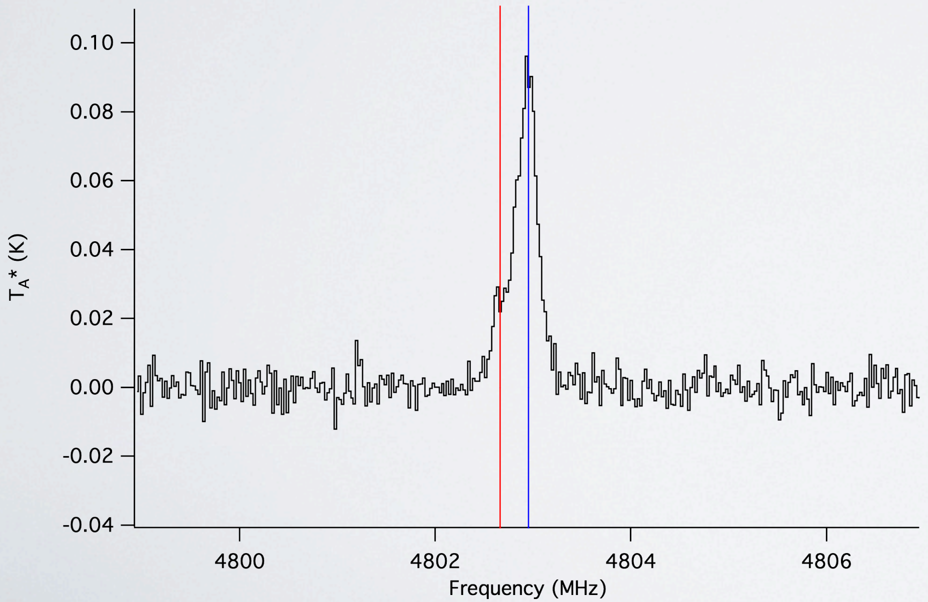
4.3 GHz	15.9 GHz
4.8 GHz	16.4 GHz
25.1 GHz	36.7 GHz
25.5 GHz	37.1 GHz
45.8 GHz	
46.3 GHz	

HNCNH Transitions

4.3 GHz	~~15.9 GHz~~
4.8 GHz	~~16.4 GHz~~
25.1 GHz	36.7 GHz
25.5 GHz	37.1 GHz
45.8 GHz	
~~46.3 GHz~~	

CARBODIIMIDE - SPECTRA





HNCNH Transitions

4.3 GHz
4.8 GHz

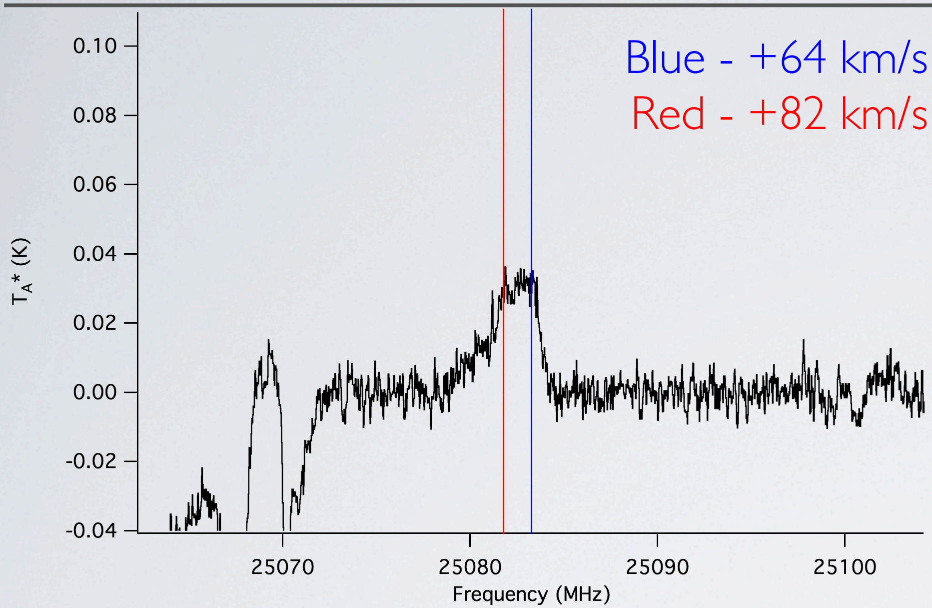
~~15.9 GHz~~
~~16.4 GHz~~

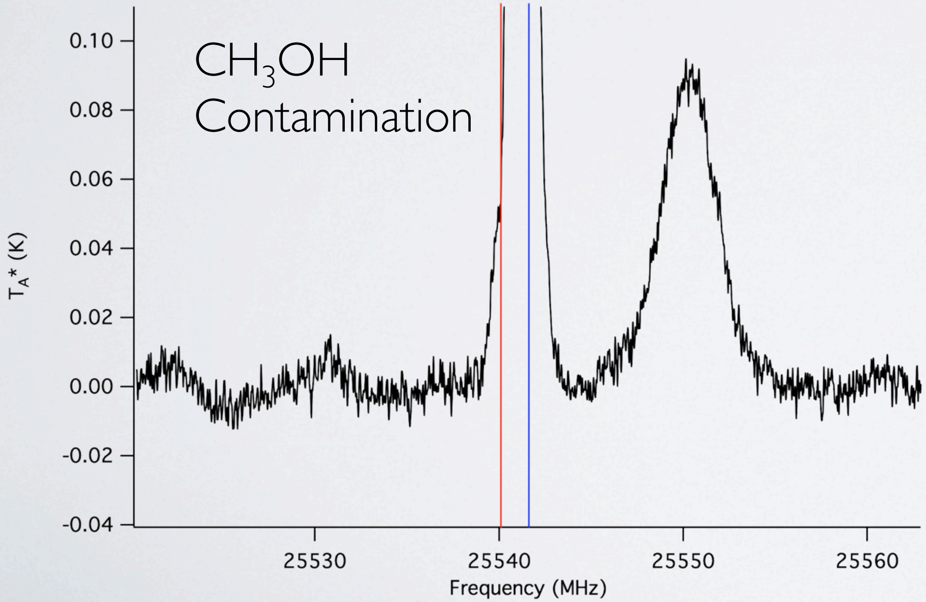
25.1 GHz
25.5 GHz

36.7 GHz
37.1 GHz

45.8 GHz
~~46.3 GHz~~

CARBODIIMIDE - SPECTRA





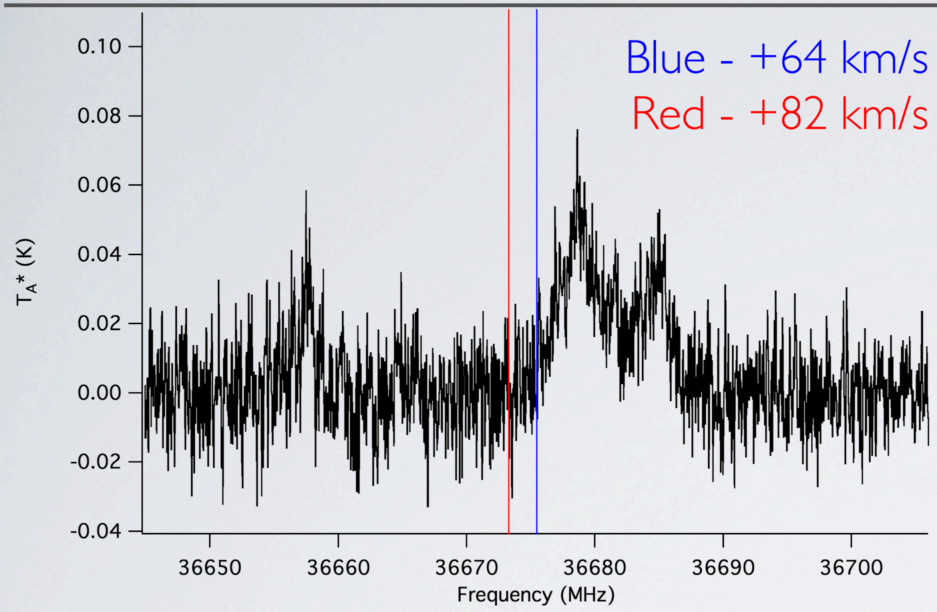
HNCNH Transitions

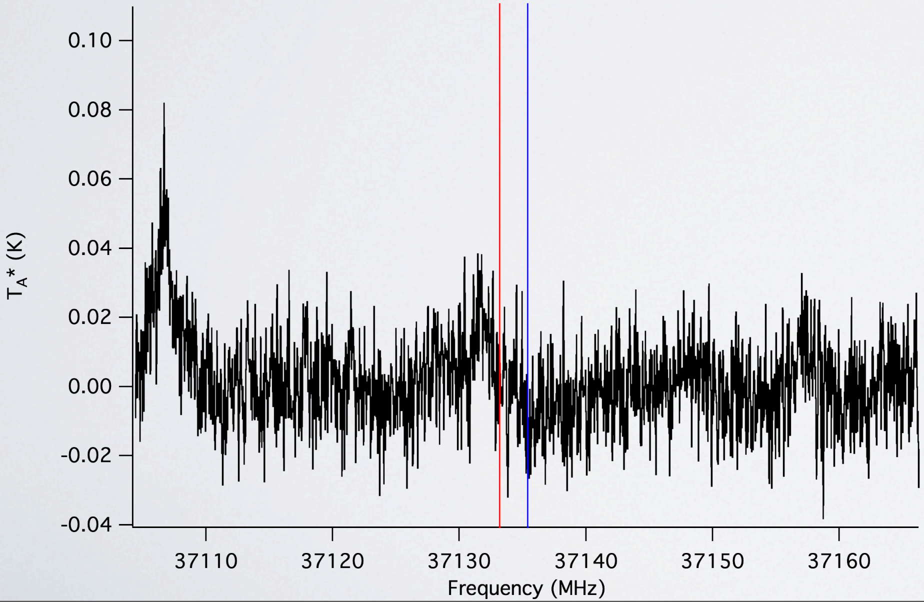
4.3 GHz ~~15.9 GHz~~
4.8 GHz ~~16.4 GHz~~

25.1 GHz 36.7 GHz
~~25.5 GHz~~ 37.1 GHz

45.8 GHz
~~46.3 GHz~~

CARBODIIMIDE - SPECTRA





HNCNH Transitions

4.3 GHz
4.8 GHz

~~15.9 GHz~~
~~16.4 GHz~~

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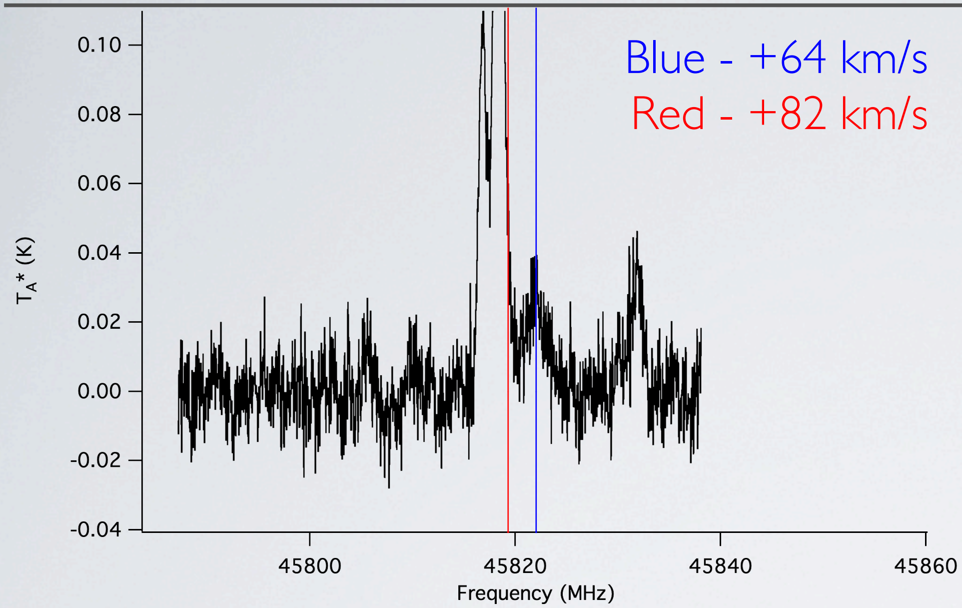
45.8 GHz
~~46.3 GHz~~

CARBODIIMIDE - SPECTRA



HNCNH Transitions

4.3 GHz
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~~15.9 GHz~~
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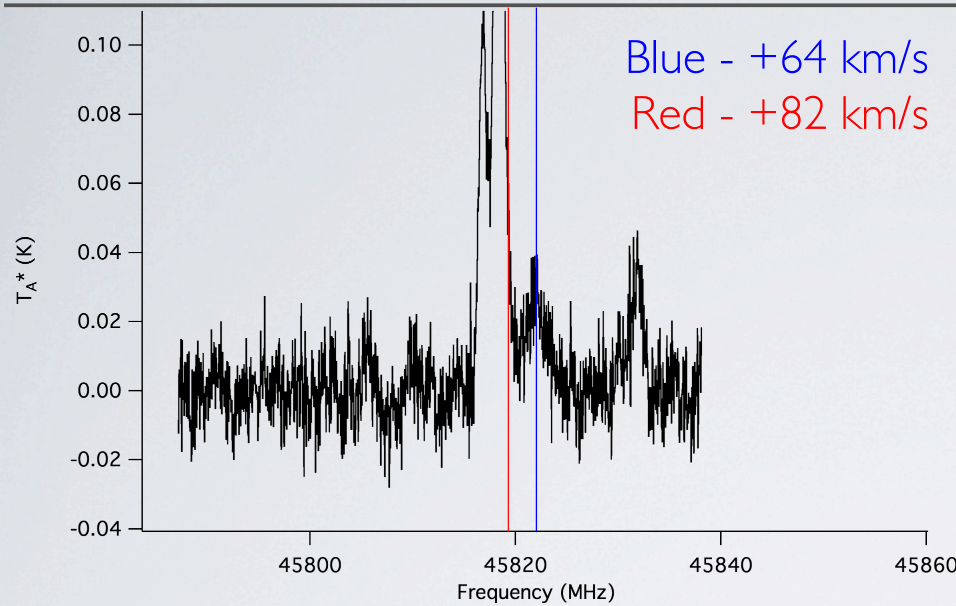
36.7 GHz
37.1 GHz

45.8 GHz
~~46.3 GHz~~

CARBODIIMIDE - SPECTRA



HNCNH Transitions

4.3 GHz
4.8 GHz

~~15.9 GHz~~
~~16.4 GHz~~

25.1 GHz
~~25.5 GHz~~

36.7 GHz
37.1 GHz

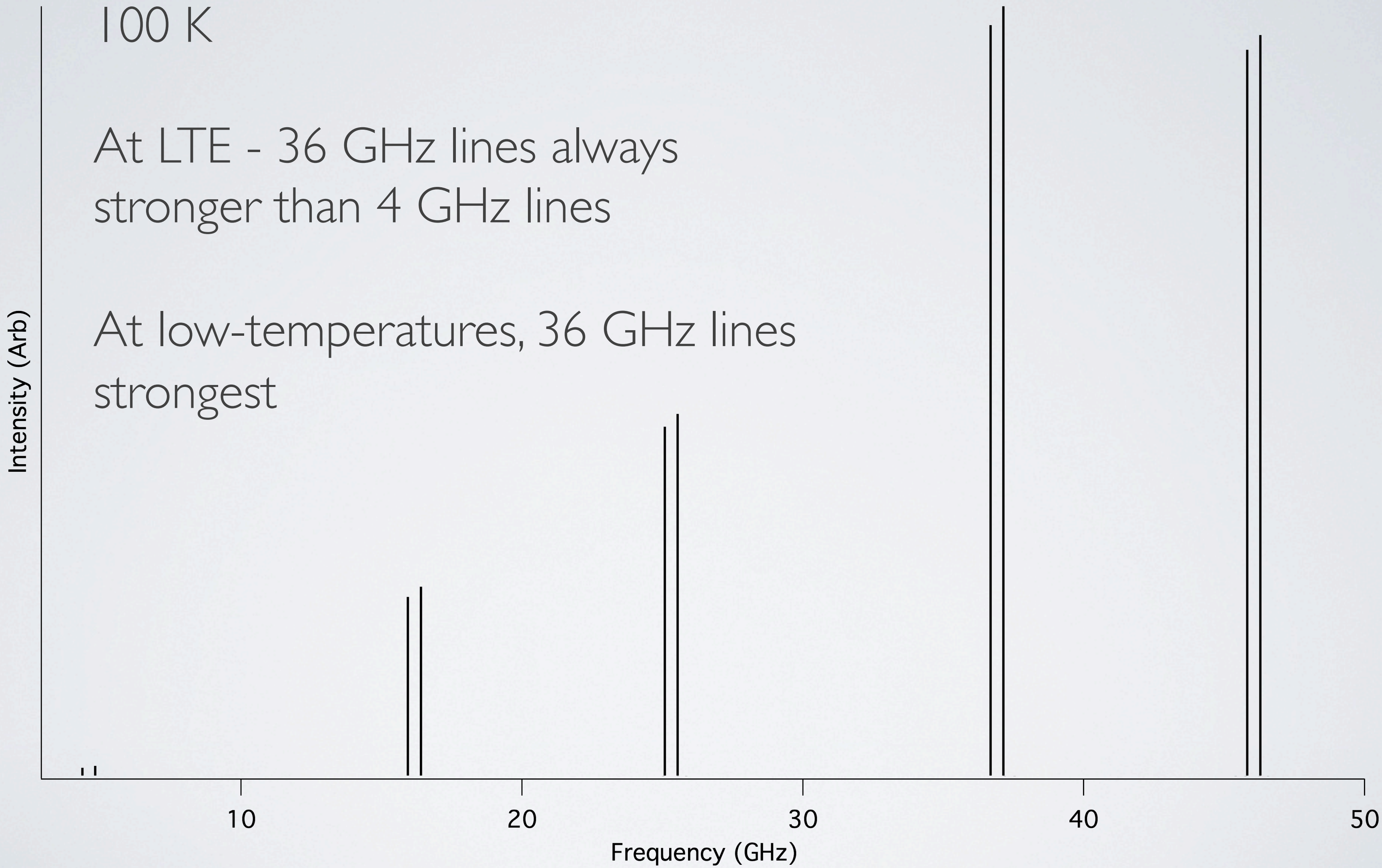
45.8 GHz
~~46.3 GHz~~

? ? ?

Once a candidate line is assigned, the assumption of optical thinness under LTE conditions allows predictions of intensities of additional confirming transitions …

Hence, a key test of the correctness of the assignment of a transitions is that any other transitions connected by favorable transition probabilities must also be present if the relative intensity predictions lead to detectable signals levels.

-Snyder et al. (2005)



100 K

At LTE - 36 GHz lines always stronger than 4 GHz lines

At low-temperatures, 36 GHz lines strongest

What is the probability that the lines at 4 GHz are the result of coincidental overlap with other species?

Neill et al., 2012, ApJ, 755, 153

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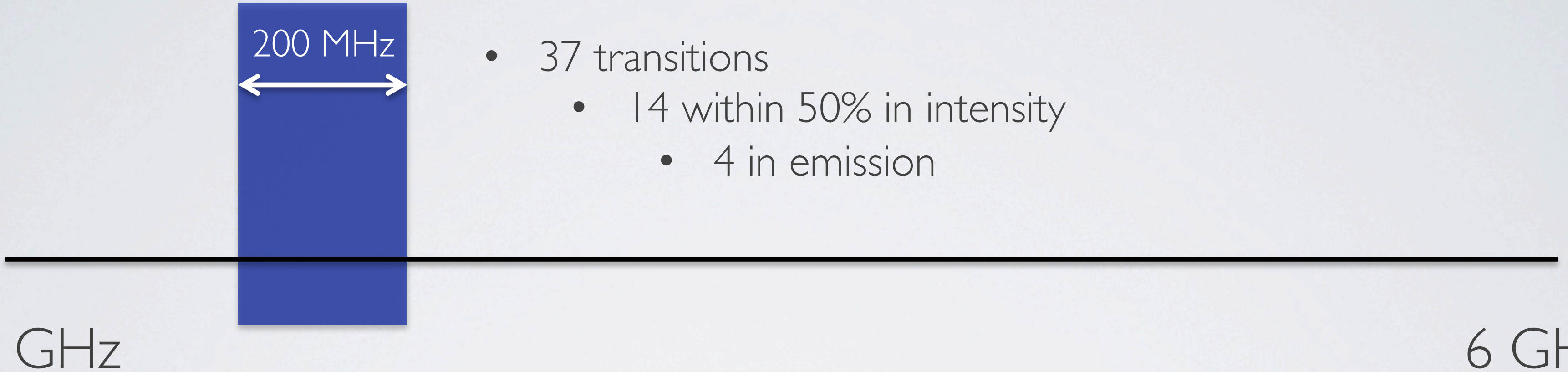
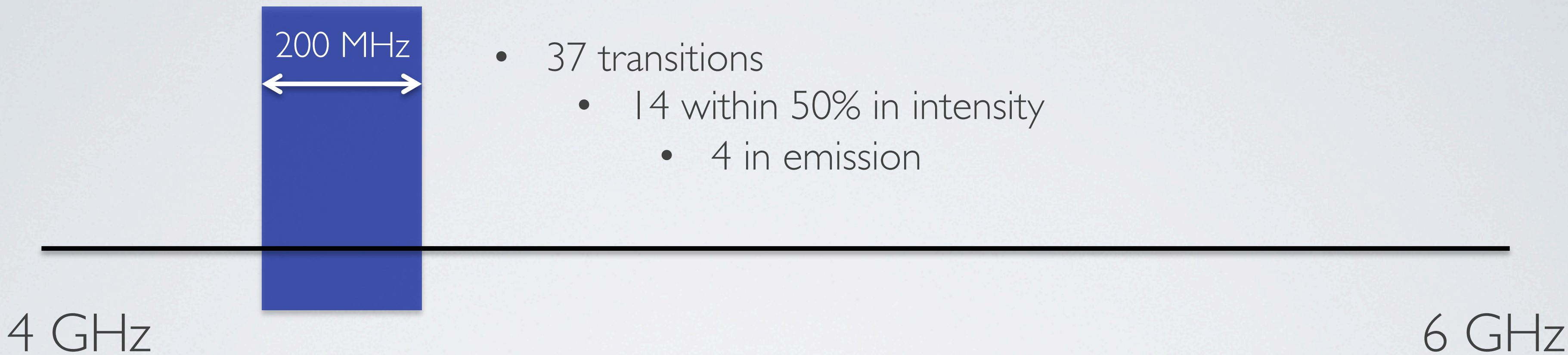


- 37 transitions
  - 14 within 50% in intensity
    - 4 in emission

Neill et al., 2012, ApJ, 755, 153

CARBODIIMIDE - PROBABILITIES

What is the probability that the lines at 4 GHz are the result of coincidental overlap with other species?



- 37 transitions
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Assume 25 km s^{-1} FWHM

Neill et al., 2012, ApJ, 755, 153

CARBODIIMIDE - PROBABILITIES

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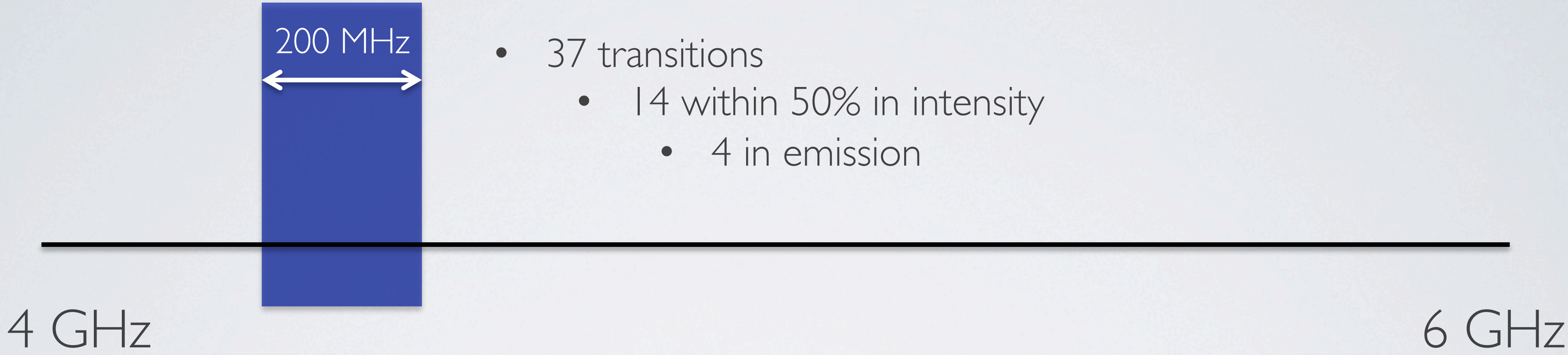
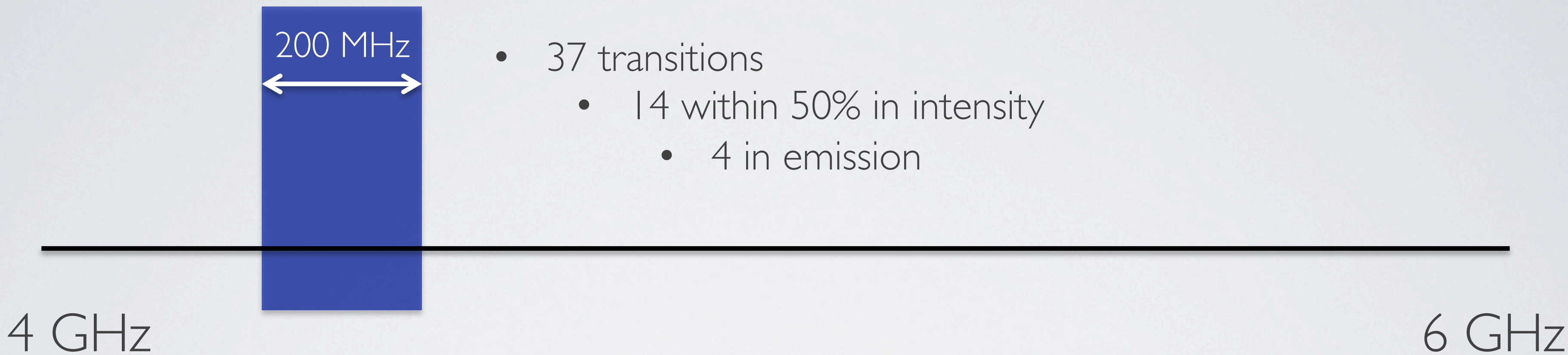


Assume 25 km s^{-1} FWHM

Probability of one line falling within one FWHM: 0.75%

Neill et al., 2012, ApJ, 755, 153

What is the probability that the lines at 4 GHz are the result of coincidental overlap with other species?



- 37 transitions
  - 14 within 50% in intensity
    - 4 in emission

Assume 25 km s^{-1} FWHM

Probability of one line falling within one FWHM: 0.75%
Probability of two lines falling within one FWHM: **0.002%**

Neill et al., 2012, ApJ, 755, 153

What is the probability that the lines at 4 GHz are the result of coincidental overlap with other species?

200 MHz

- 37 transitions
  - 4 in emission

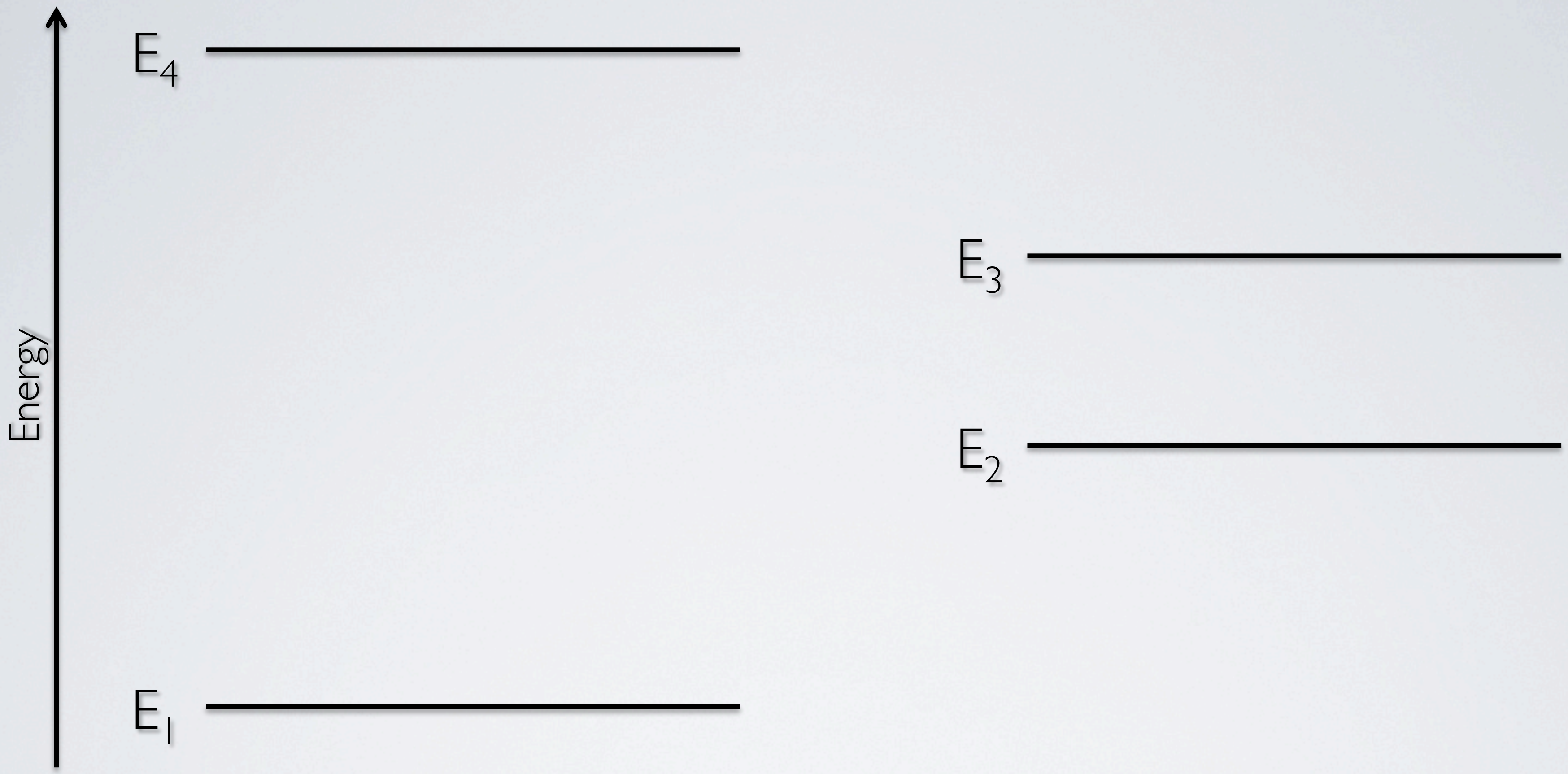
Convincing, but what about the missing transitions?

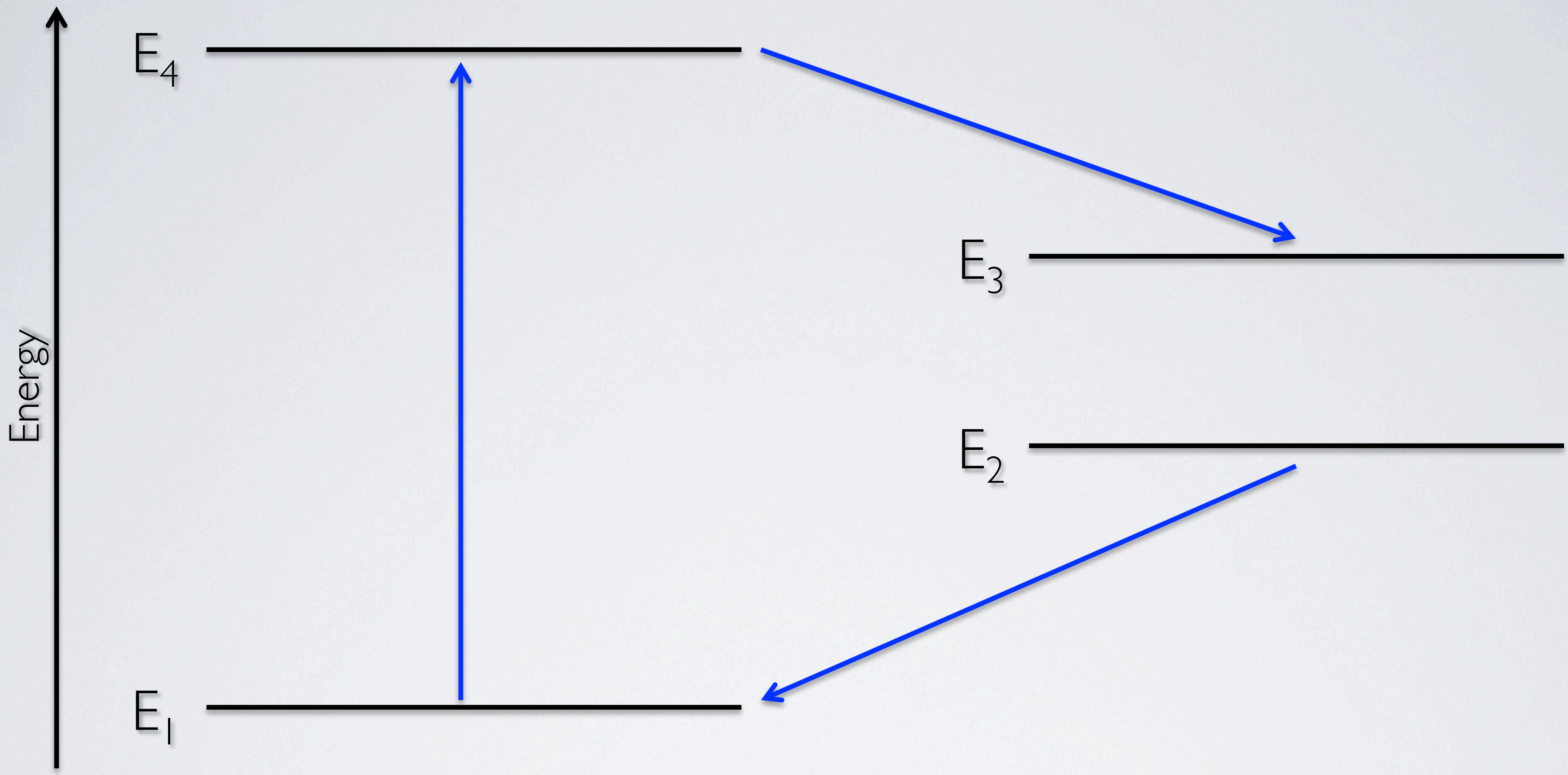
4 GHz 6 GHz

Assume 25 km s^{-1} FWHM

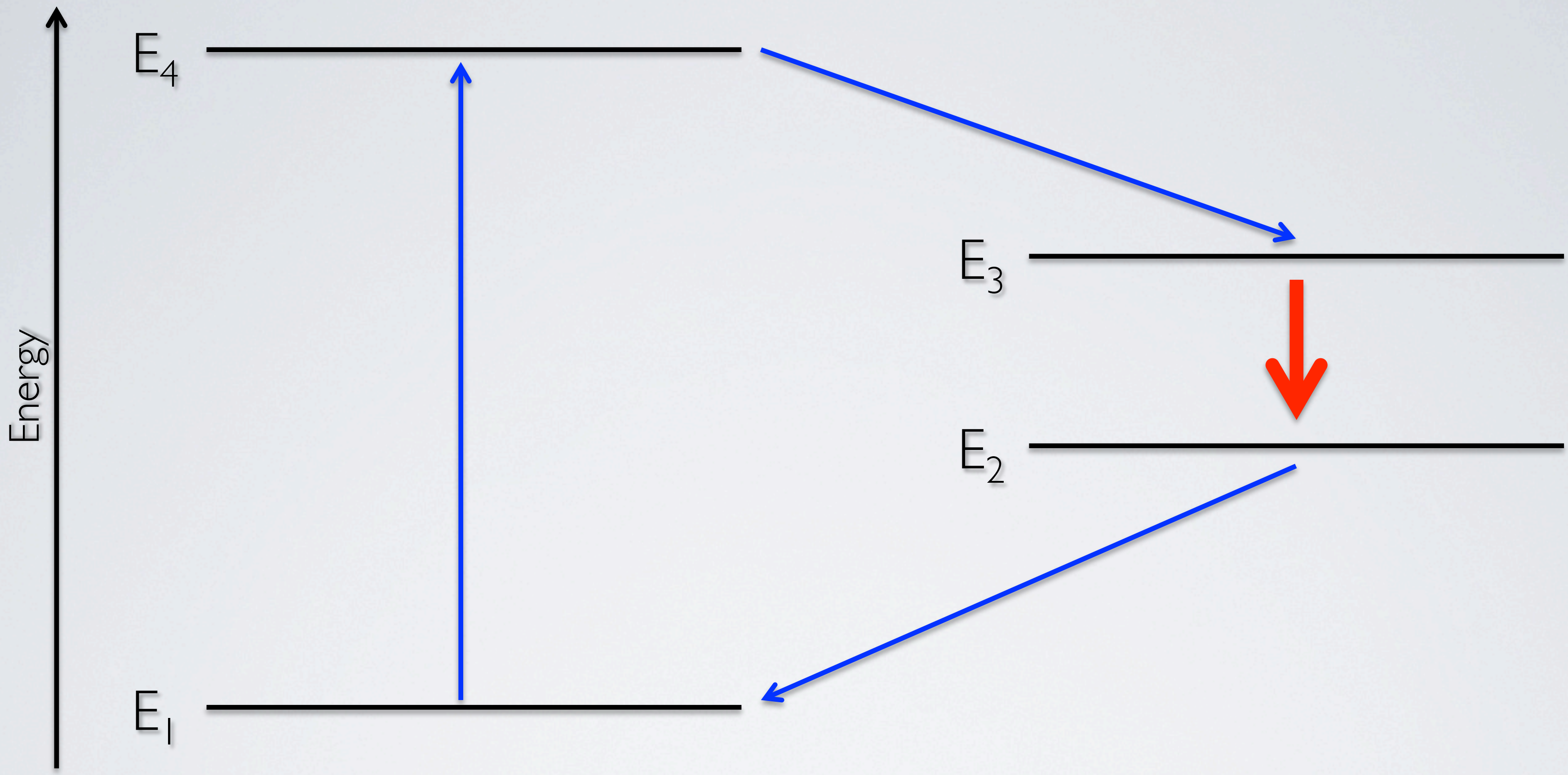
Probability of one line falling within one FWHM: 0.75%
Probability of two lines falling within one FWHM: **0.002%**

Neill et al., 2012, ApJ, 755, 153

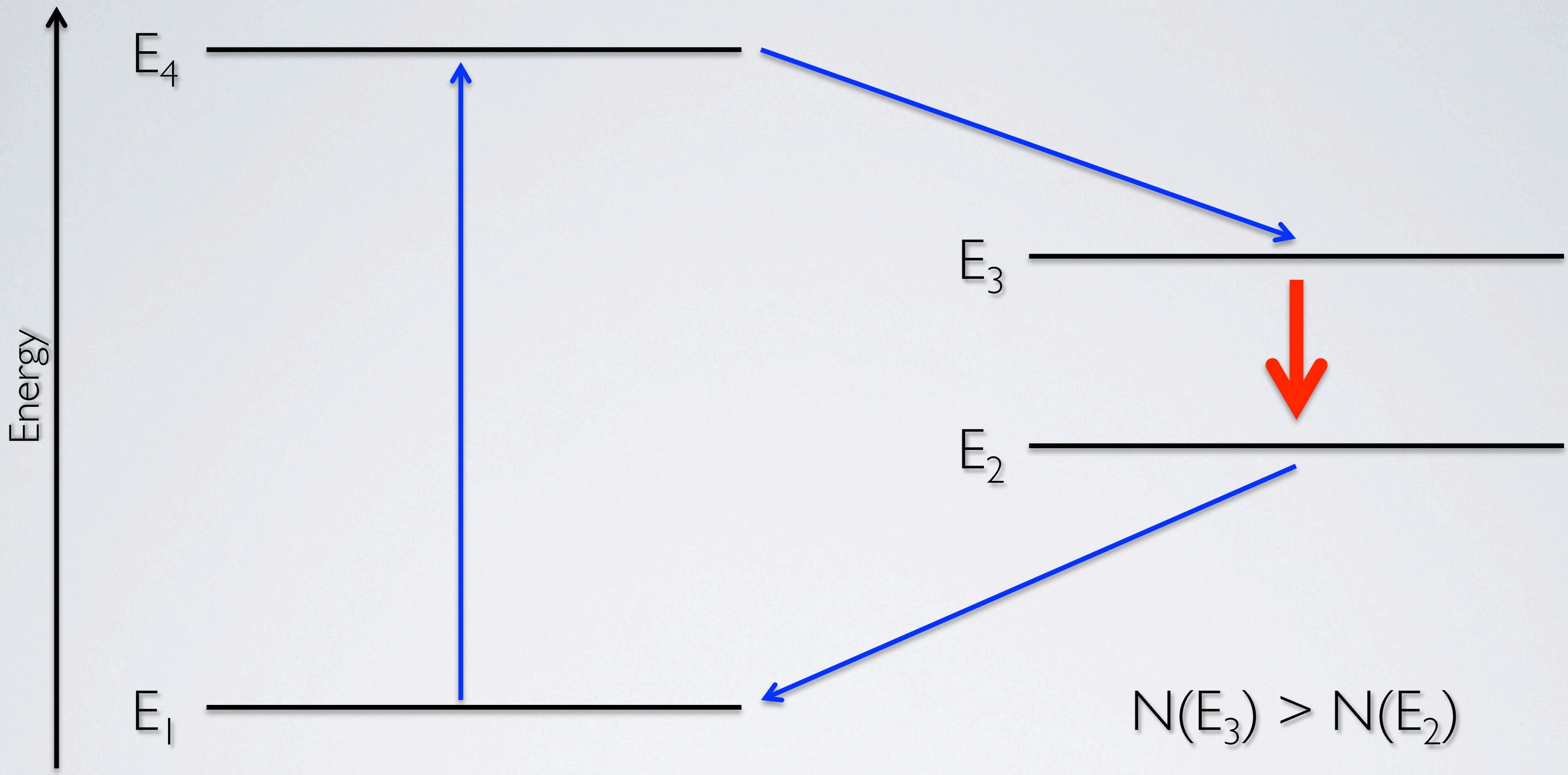

Energy
E_4
E_3
E_2
E_1



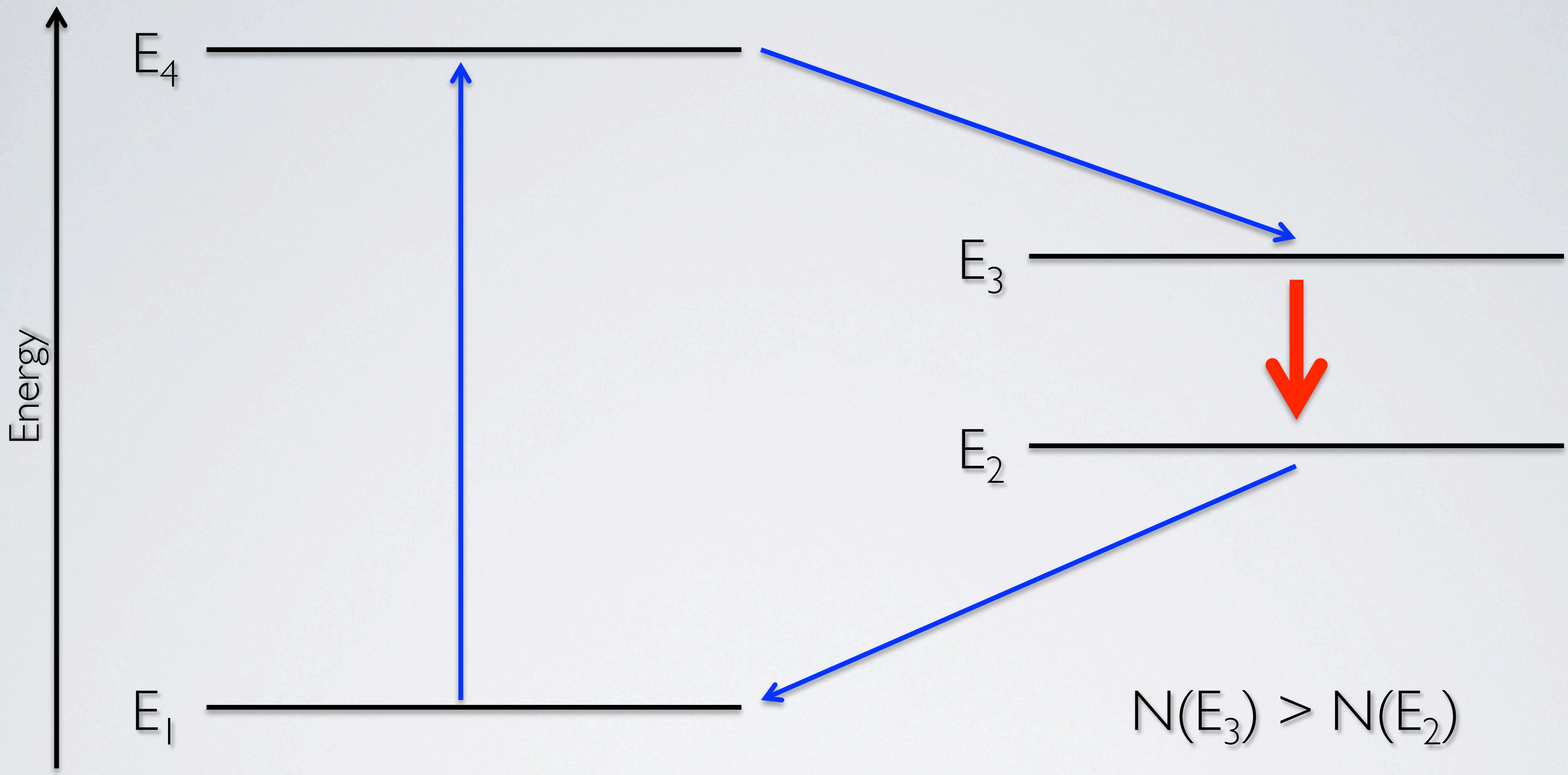
Energy
E4
E3
E2
E1



Energy
E4
E3
E2
E1



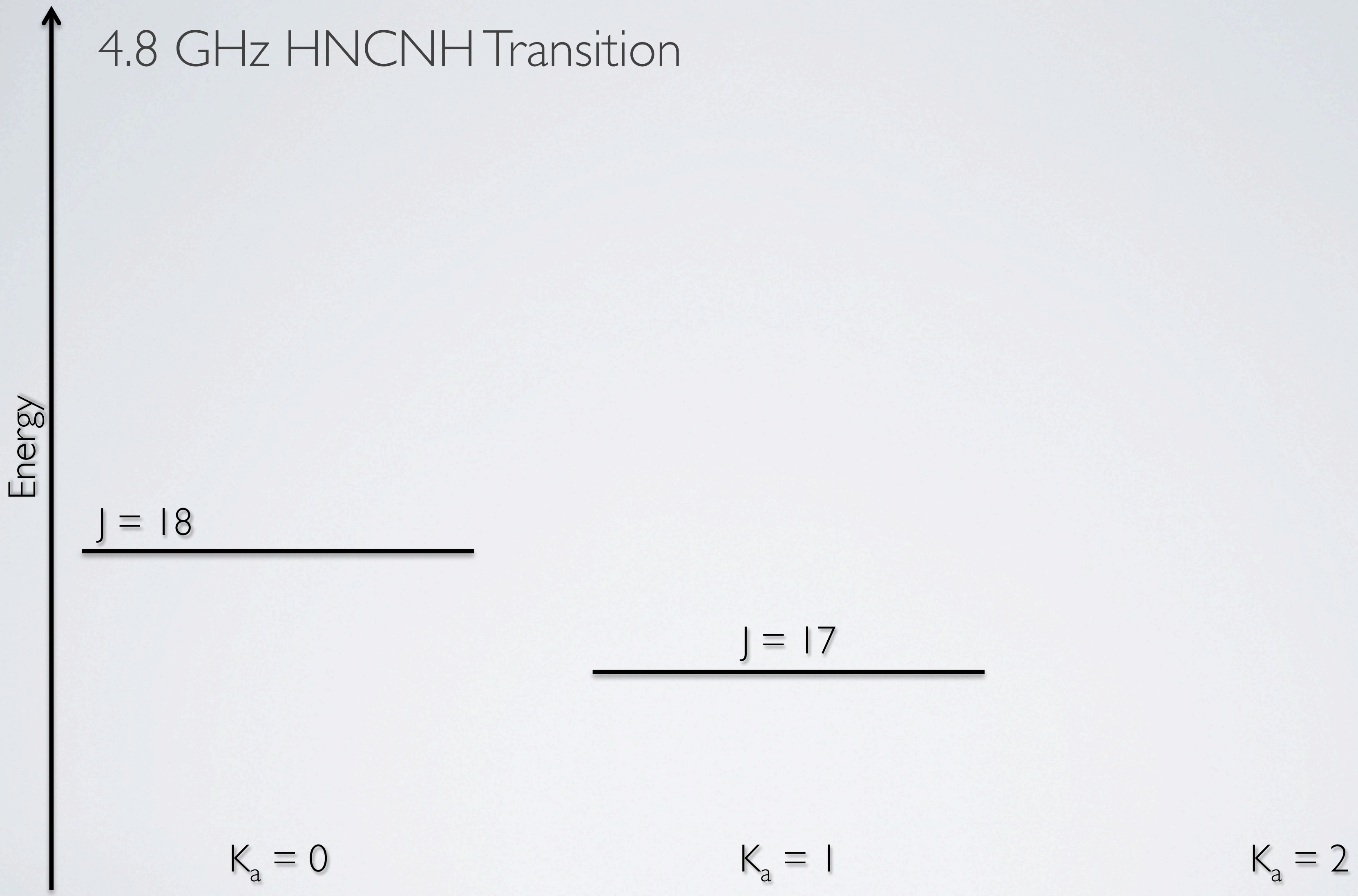
$N(E_3) > N(E_2)$



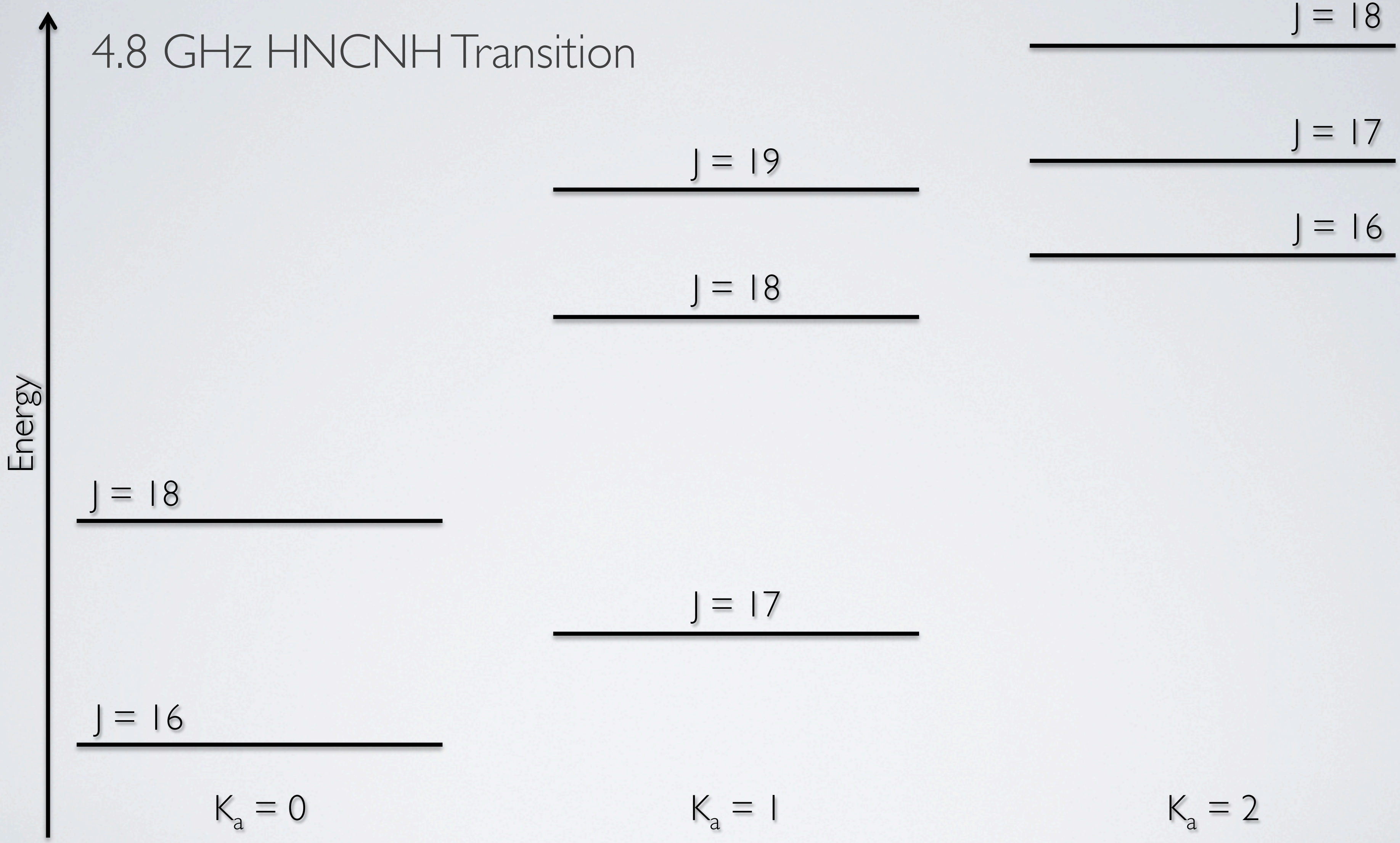
Stimulated Emission → Coherent Emission → M(L)ASING

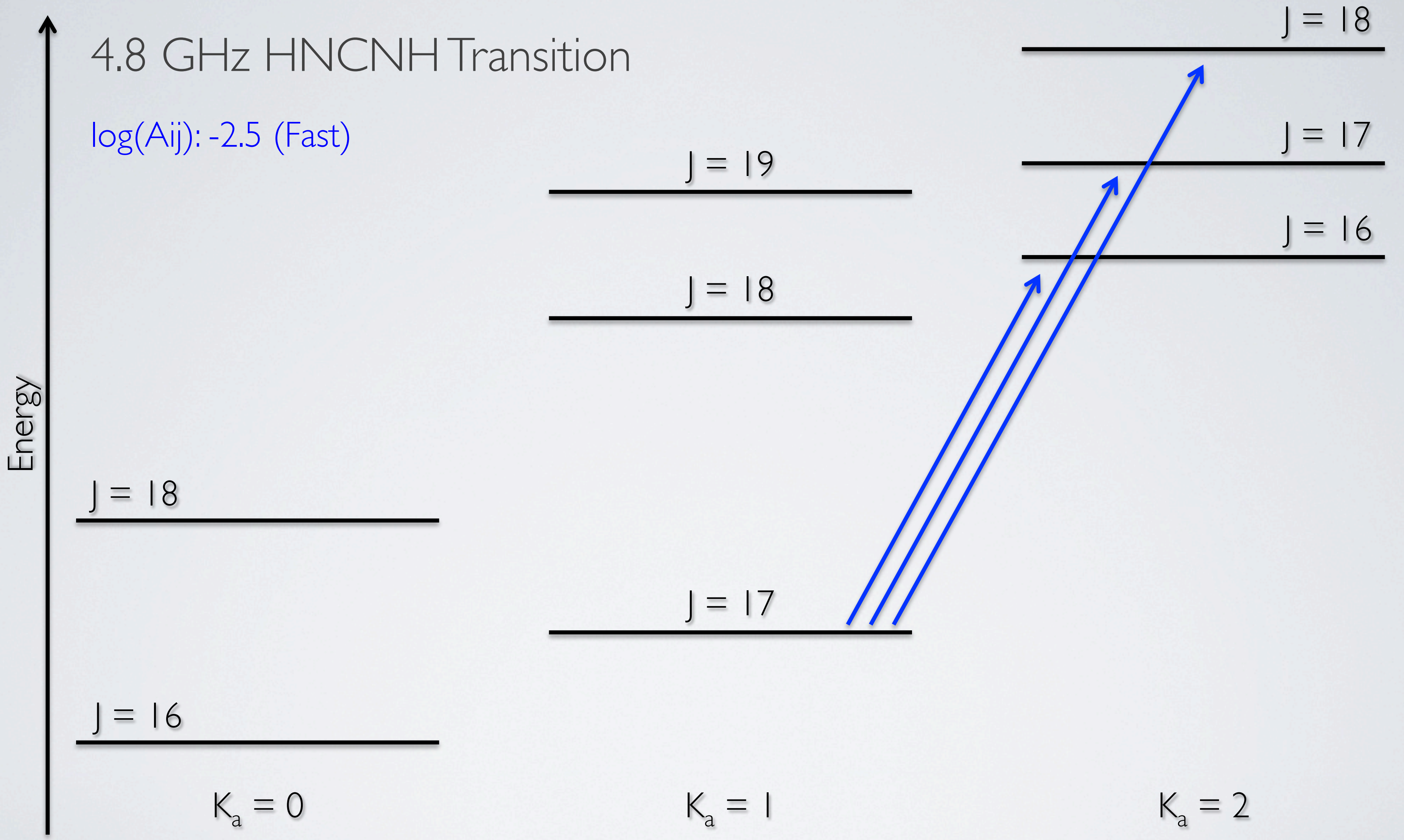
CARBODIIMIDE - ENERGY LEVELS

4.8 GHz HNCNH Transition

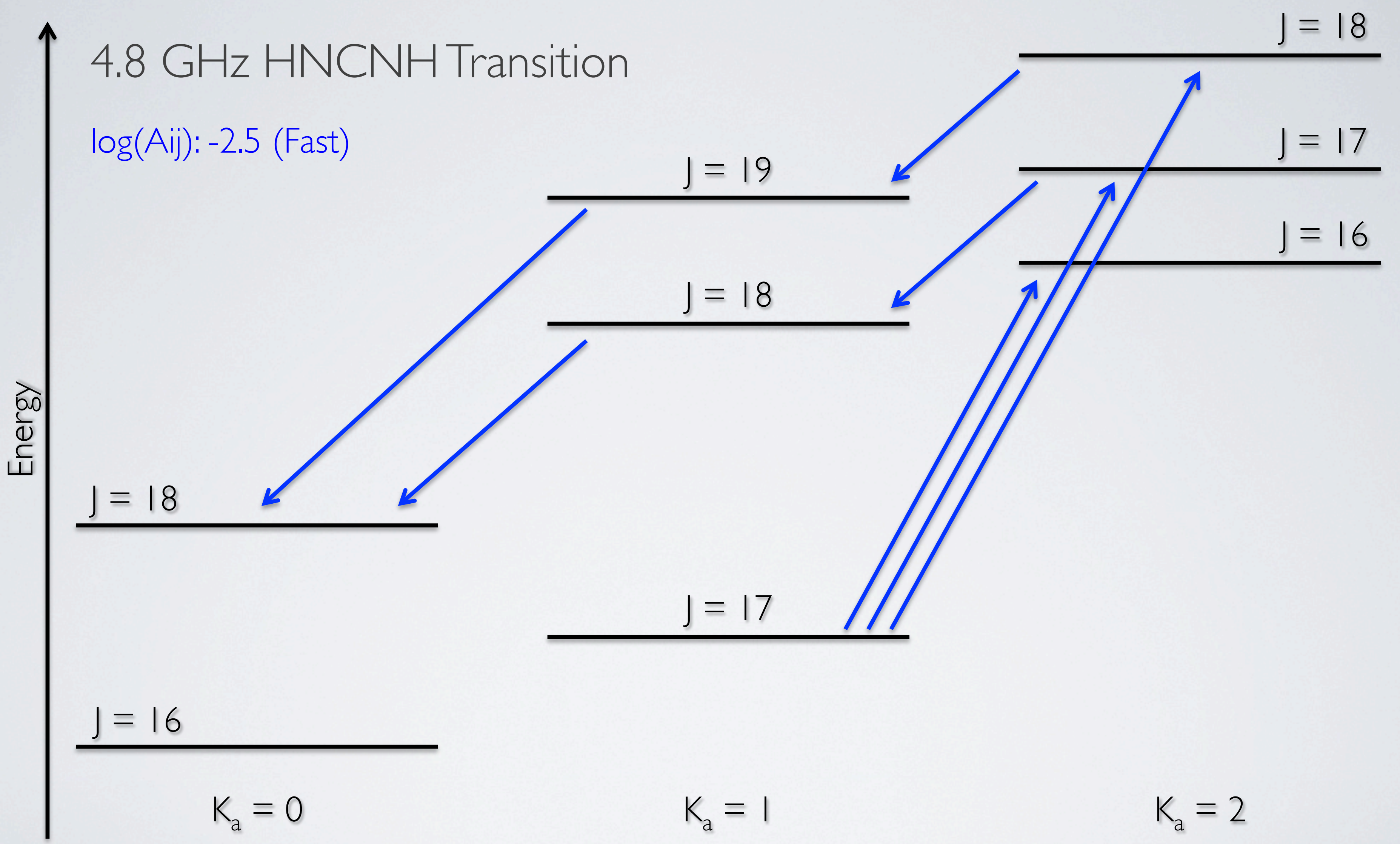


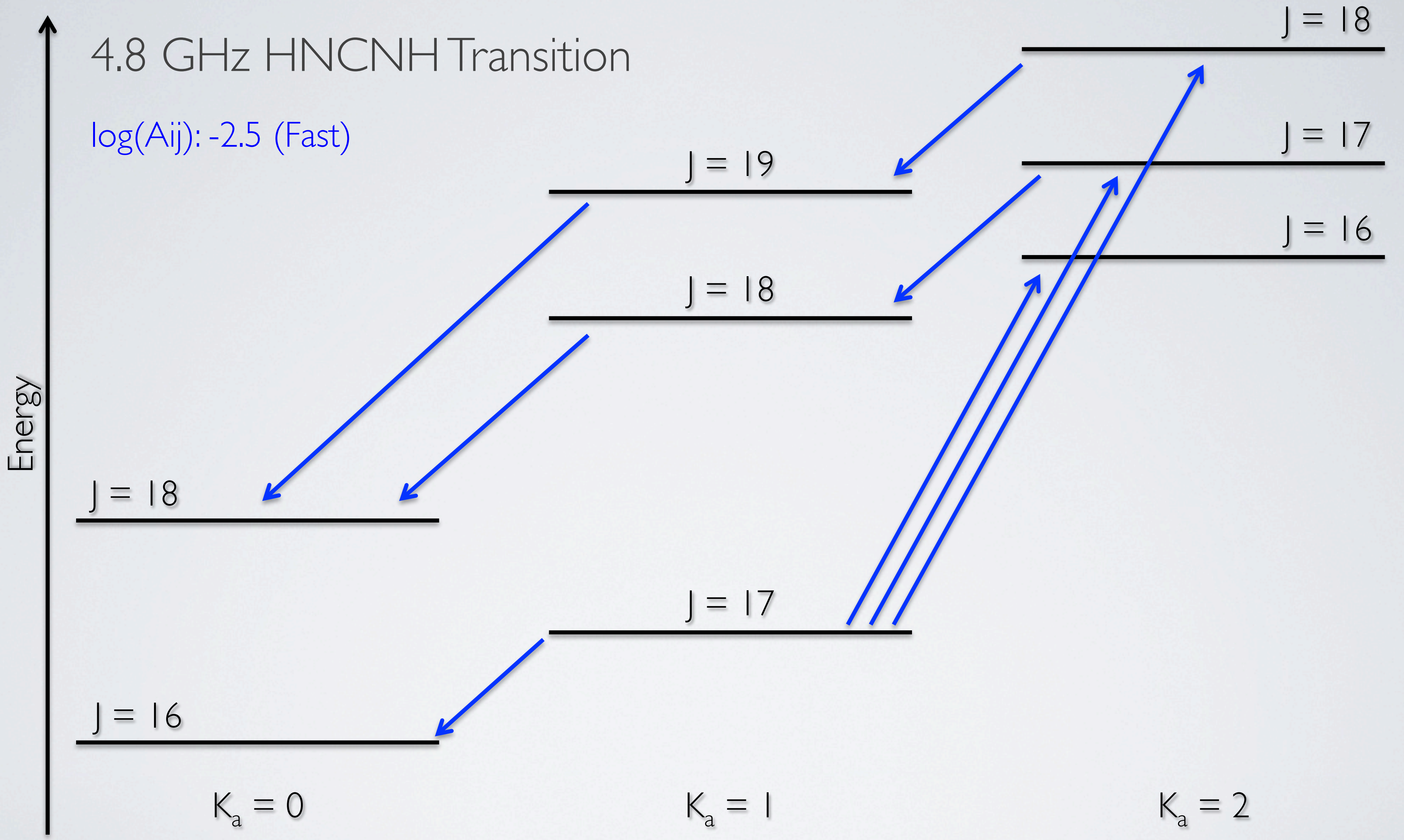
CARBODIIMIDE - ENERGY LEVELS



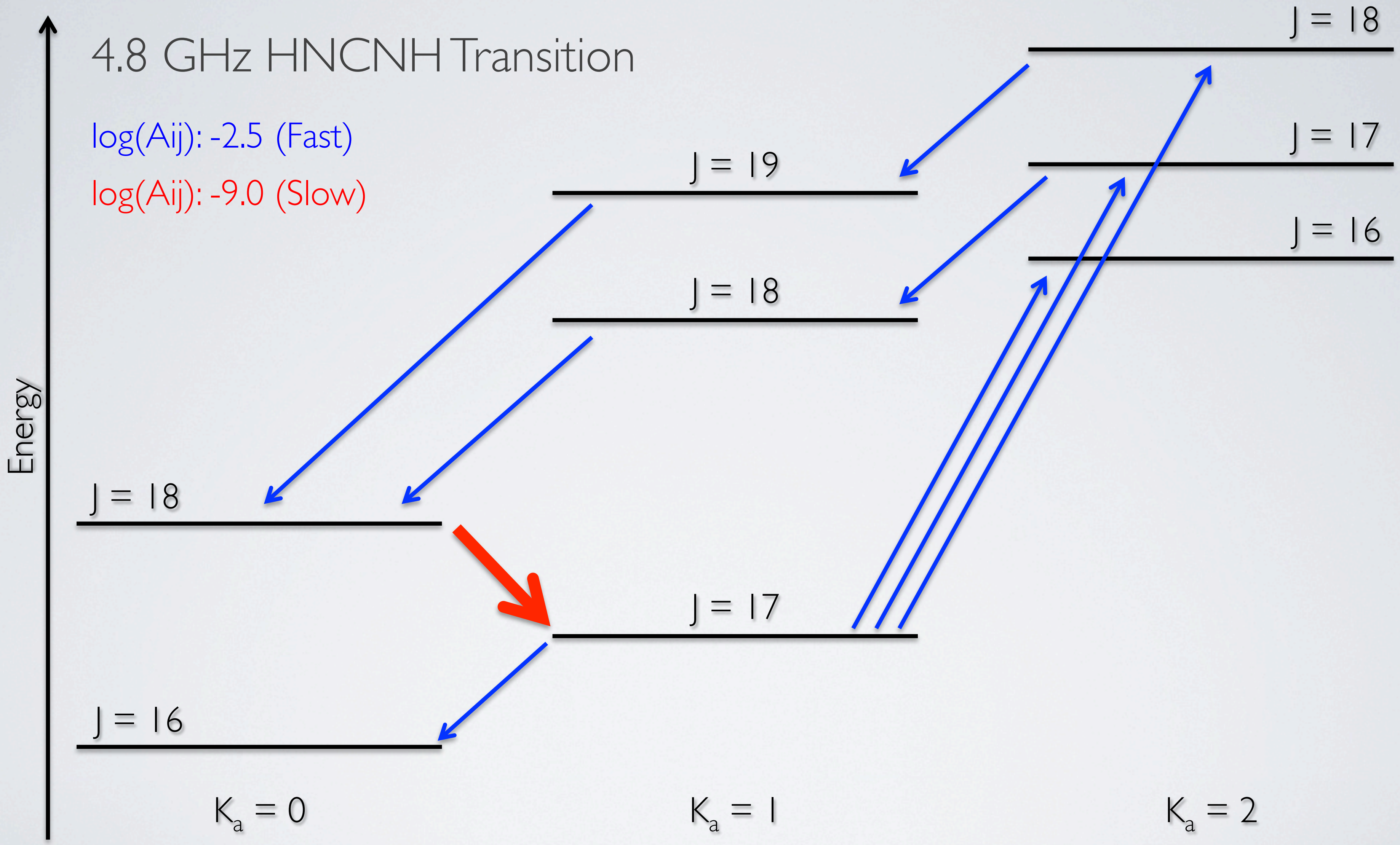

4.8 GHz HNCNH Transition
log(Aij): -2.5 (Fast)
Energy
J = 18
J = 16
J = 19
J = 18
J = 17
J = 18
J = 17
J = 16
Ka = 0
Ka = 1
Ka = 2

CARBODIIMIDE - ENERGY LEVELS



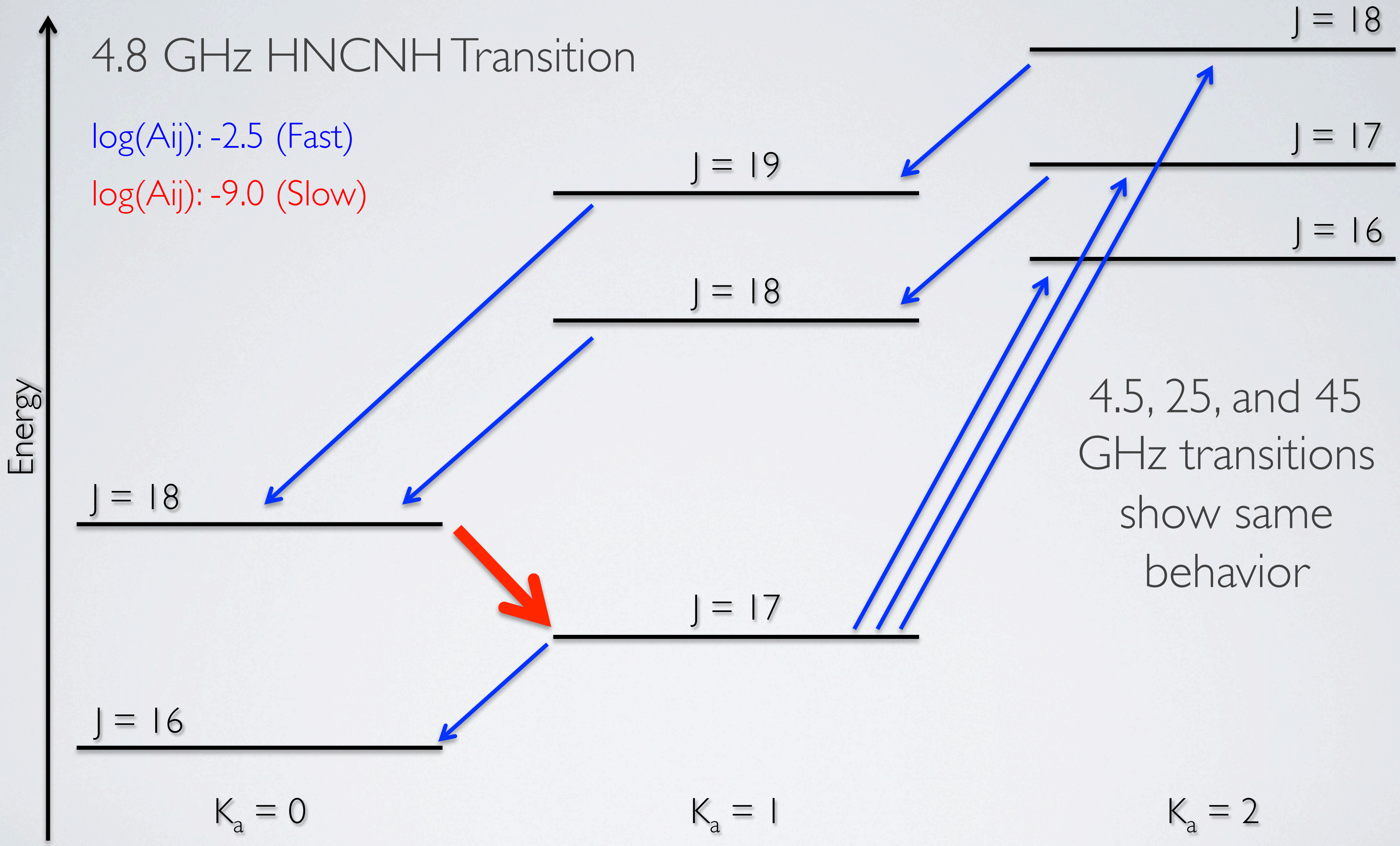


4.8 GHz HNCNH Transition
log(Aij): -2.5 (Fast)
Energy
J = 18
J = 16
J = 19
J = 18
J = 17
J = 18
J = 17
J = 16
K
a
= 0
K
a
= 1
K
a
= 2



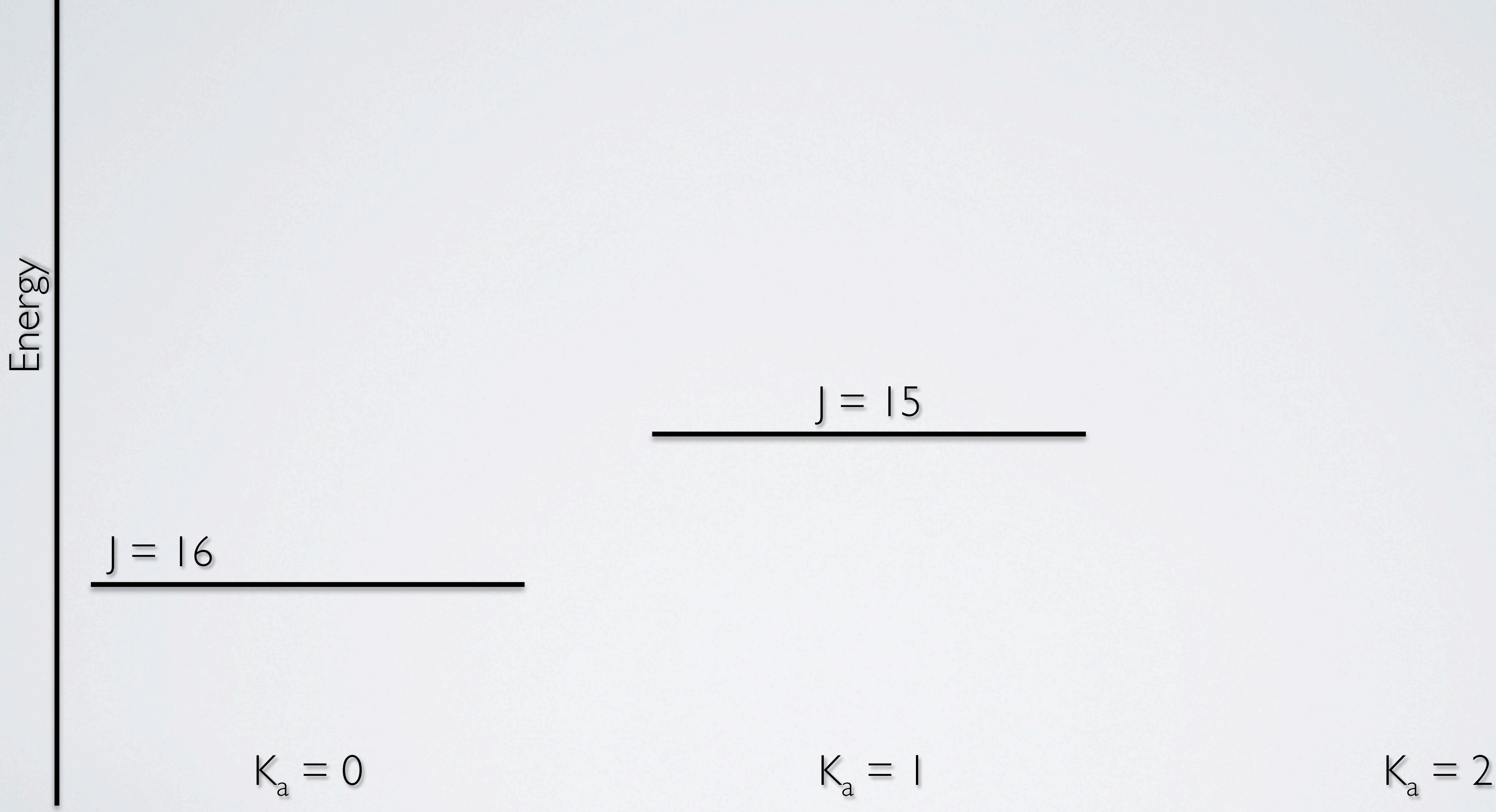
4.8 GHz HNCNH Transition
log(Aij): -2.5 (Fast)
log(Aij): -9.0 (Slow)
Energy
J = 18
J = 16
J = 19
J = 18
J = 17
J = 18
J = 17
J = 16
K$_a$ = 0
K$_a$ = 1
K$_a$ = 2

CARBODIIMIDE - ENERGY LEVELS



36.6 GHz HNCNH Transition

log(Aij): -2.5 (Fast)



36.6 GHz HNCNH Transition

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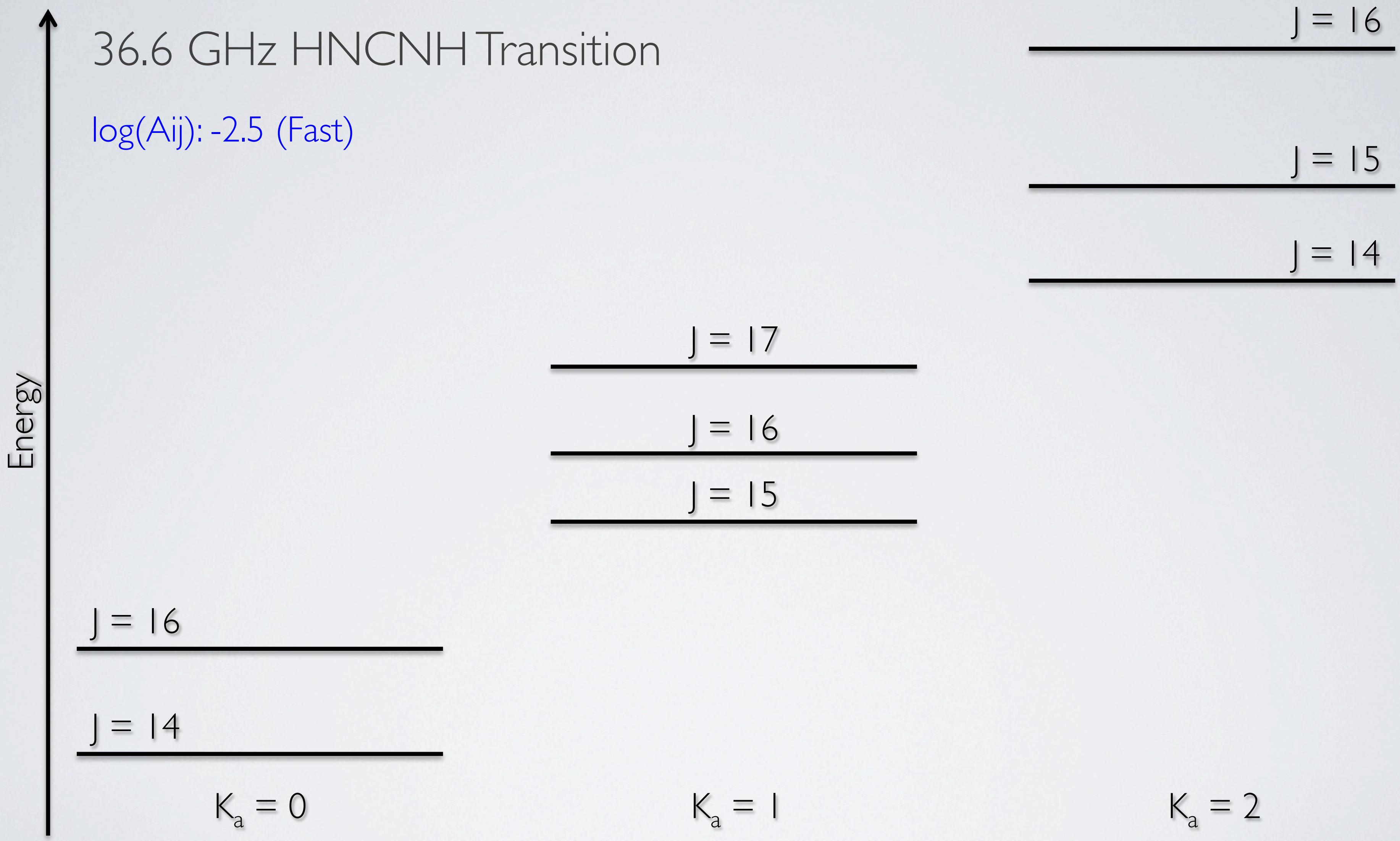
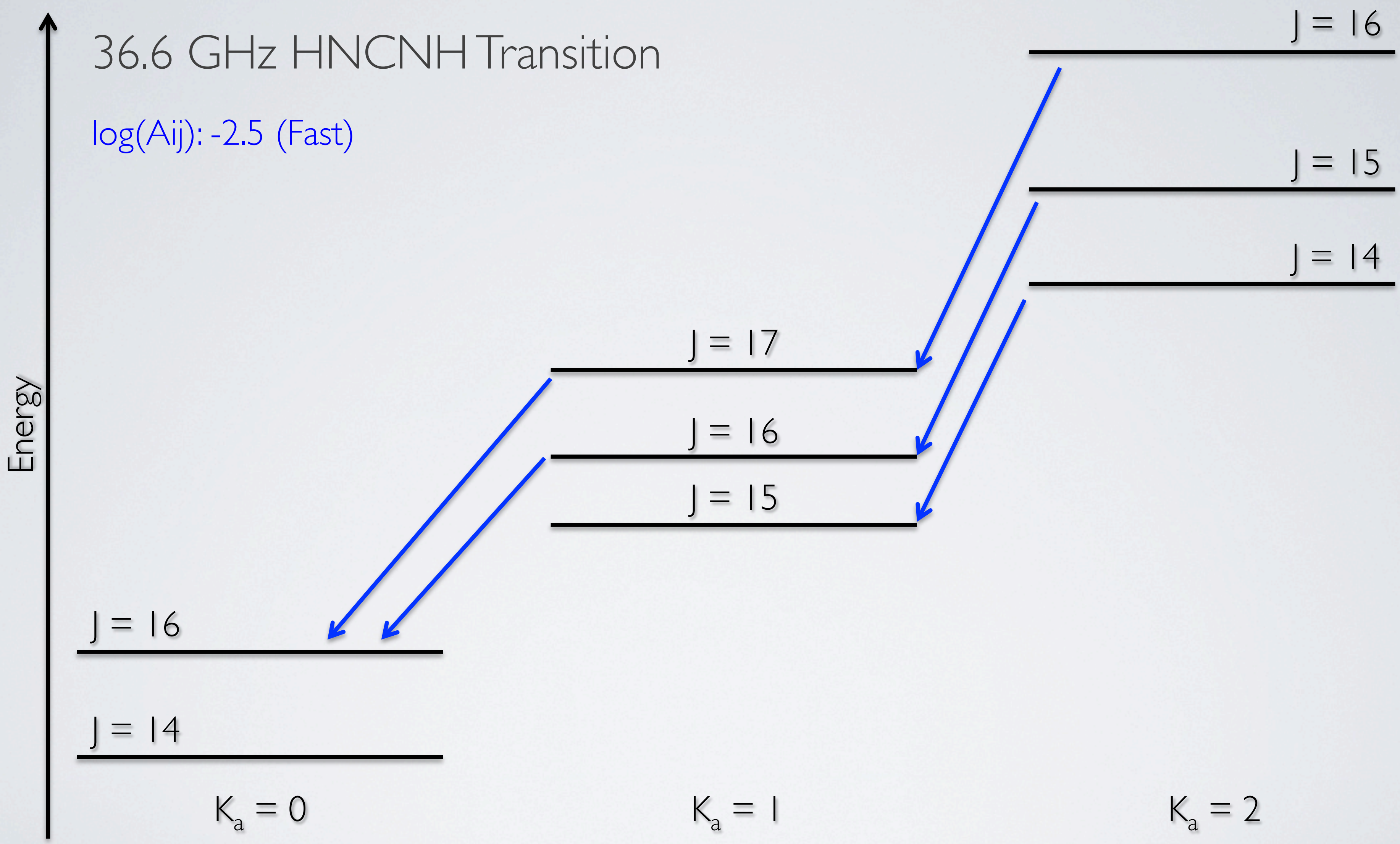
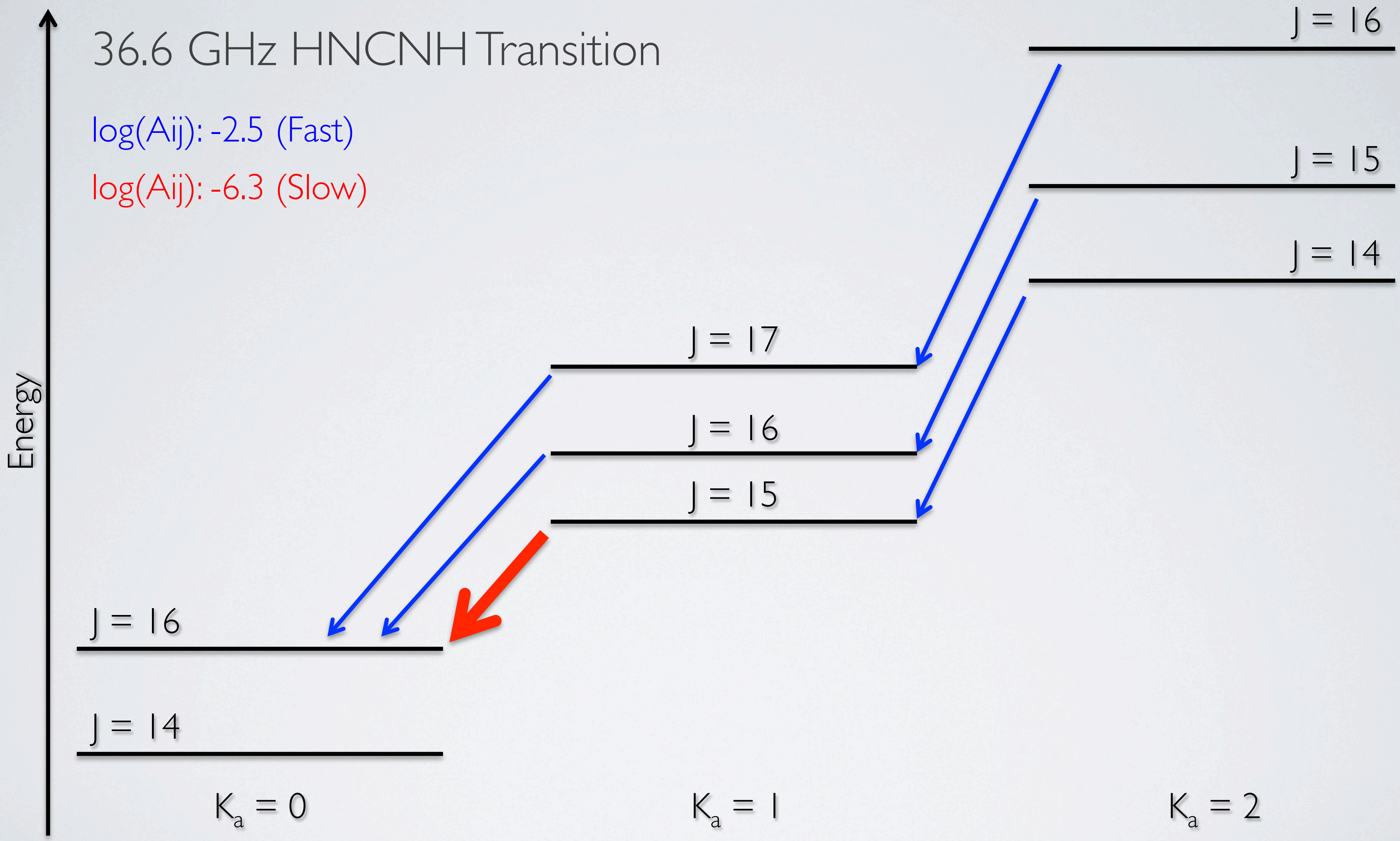
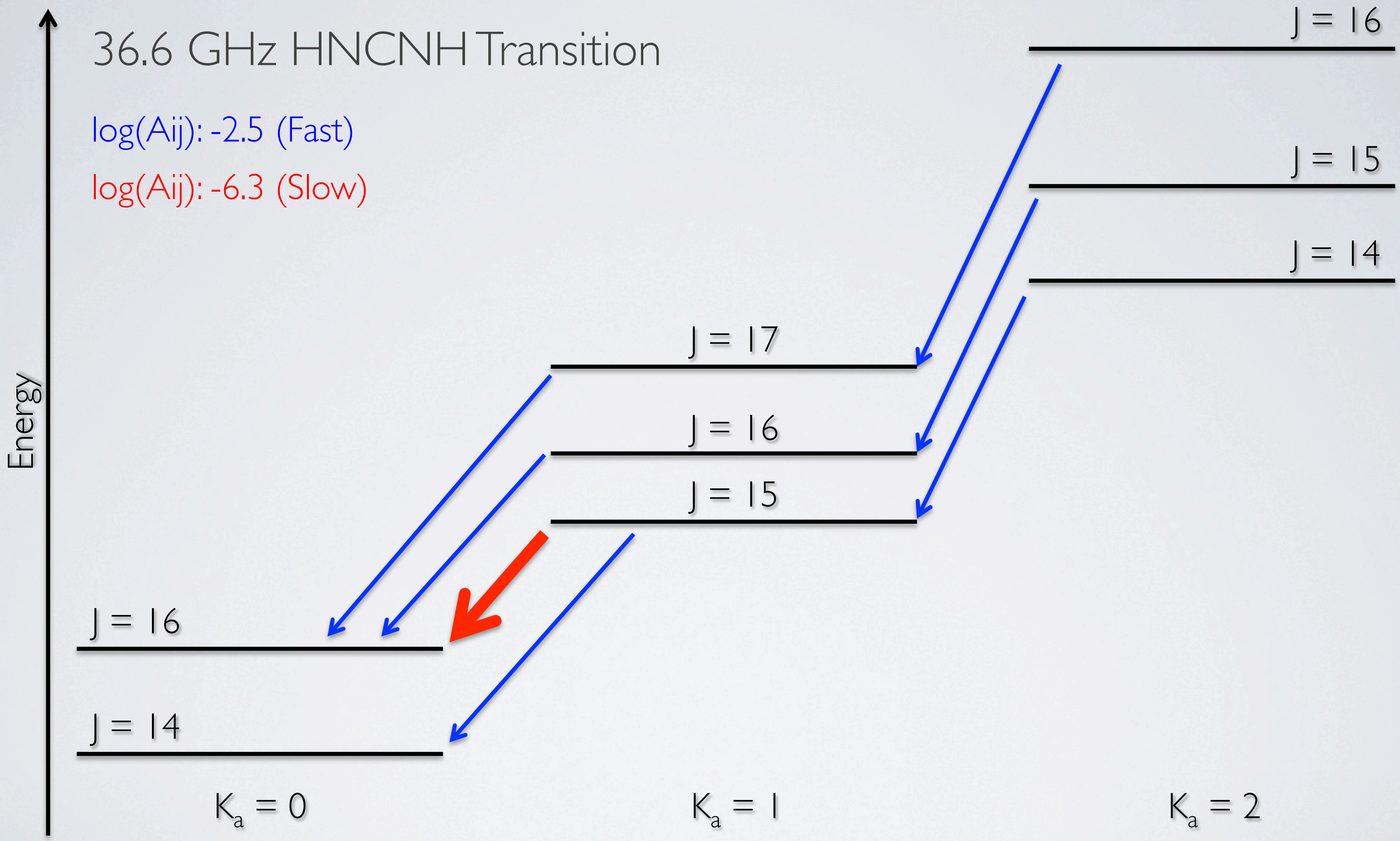



36.6 GHz HNCNH Transition
log(Aij): -2.5 (Fast)
Energy
J = 16
J = 15
J = 14
J = 17
J = 16
J = 15
J = 16
J = 14
$K_a = 0$
$K_a = 1$
$K_a = 2$


36.6 GHz HNCNH Transition
log(Aij): -2.5 (Fast)
log(Aij): -6.3 (Slow)
Energy
J = 16
J = 15
J = 14
J = 17
J = 16
J = 15
J = 16
J = 14
Ka = 0
Ka = 1
Ka = 2



36.6 GHz HNCNH Transition
log(Aij): -2.5 (Fast)
log(Aij): -6.3 (Slow)
Energy
J = 16
J = 15
J = 14
J = 17
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J = 15
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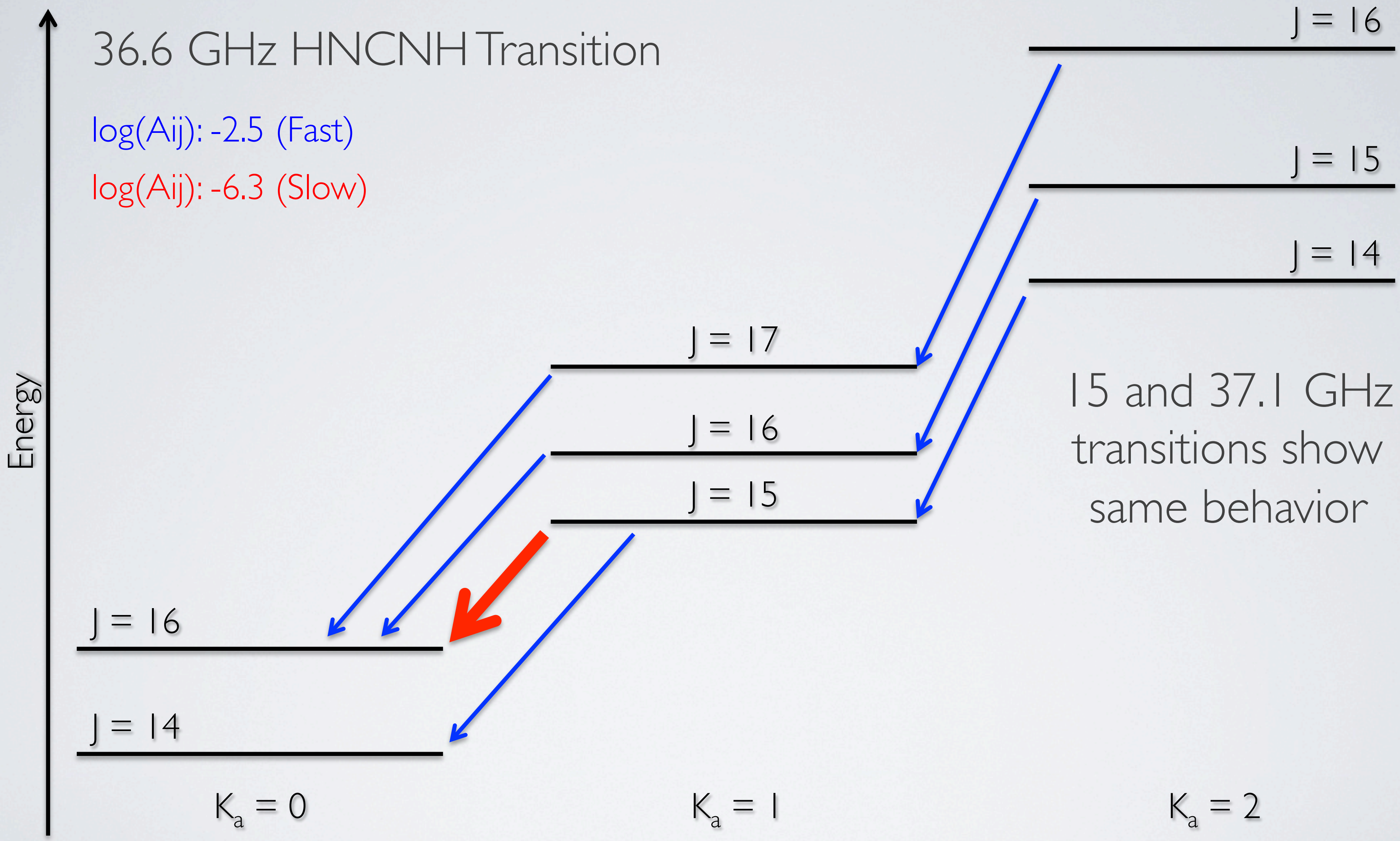
J = 14
K_a = 0
K_a = 1
K_a = 2

CARBODIIMIDE - ENERGY LEVELS



Transitions	Population Inversion?	T_A^* (mK) Observed
4 GHz	Yes	85
25 GHz	Yes	27
36 GHz	No	< 11
45 GHz	Yes	25

The 36 GHz lines aren't masing - can we see them at LTE?

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4 GHz	Yes	85
25 GHz	Yes	27
36 GHz	No	< 11
45 GHz	Yes	25

The 36 GHz lines aren't masing - can we see them at LTE?

Transitions	Population Inversion?	T_A^* (mK) Observed	T_A^* (mK) (2×10^{13} cm^{-2})
4 GHz	Yes	85	0.1
25 GHz	Yes	27	0.8
36 GHz	No	< 11	1.4
45 GHz	Yes	25	0.9
			80 K

What if the 45 GHz transition is actually thermal, not masing?

Transitions	Population Inversion?	T_A^* (mK) Observed	T_A^* (mK) (2×10^{13} cm^{-2})
4 GHz	Yes	85	0.1
25 GHz	Yes	27	0.8
36 GHz	No	< 11	1.4
45 GHz	Yes	25	0.9
			80 K

What if the 45 GHz transition is actually thermal, not masing?

Transitions	Population Inversion?	T_A^* (mK) Observed	T_A^* (mK) (2×10^{13} cm^{-2})	T_A^* (mK) (5×10^{14} cm^{-2})
4 GHz	Yes	85	0.1	3.8
25 GHz	Yes	27	0.8	23
36 GHz	No	< 11	1.4	39
45 GHz	Yes	25	0.9	25
			80 K	80 K

CARBODIIMIDE - CONCLUSIONS

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A new methodology for searching for very low-abundance, but important molecular species.

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Take Home Message

When searching for a new molecular species, always check energy levels for possibility of masing

Interstellar Carbodiimide