Infia Software

Computer program for Interactive spectrum analysis

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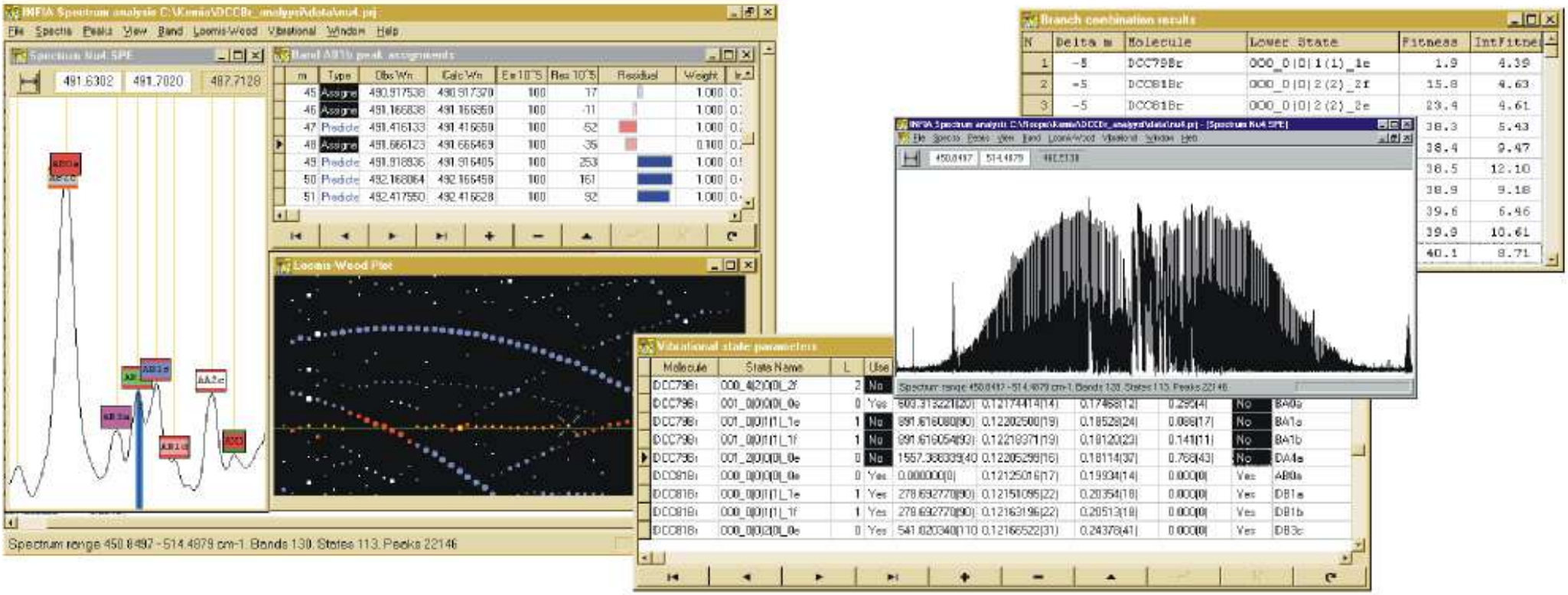
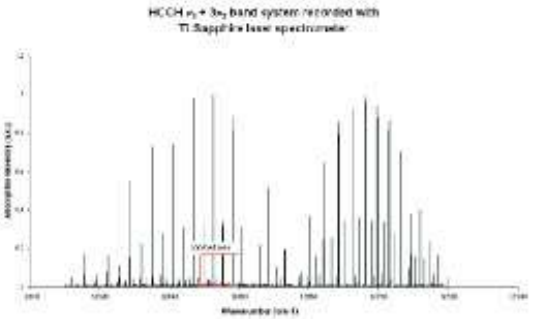


Why analyse spectra?

1. True molecular properties

2. High resolution Laser / FTIR spectrometers



3. Infrared vibration-rotation spectrum

4. Spectrum analysis

5. Molecular geometry & force field

Applications

Bulk matrial properties

Reaction dynamics simulations

Thermodynamics

Energy levels

Linear molecule vibration-rotation energy

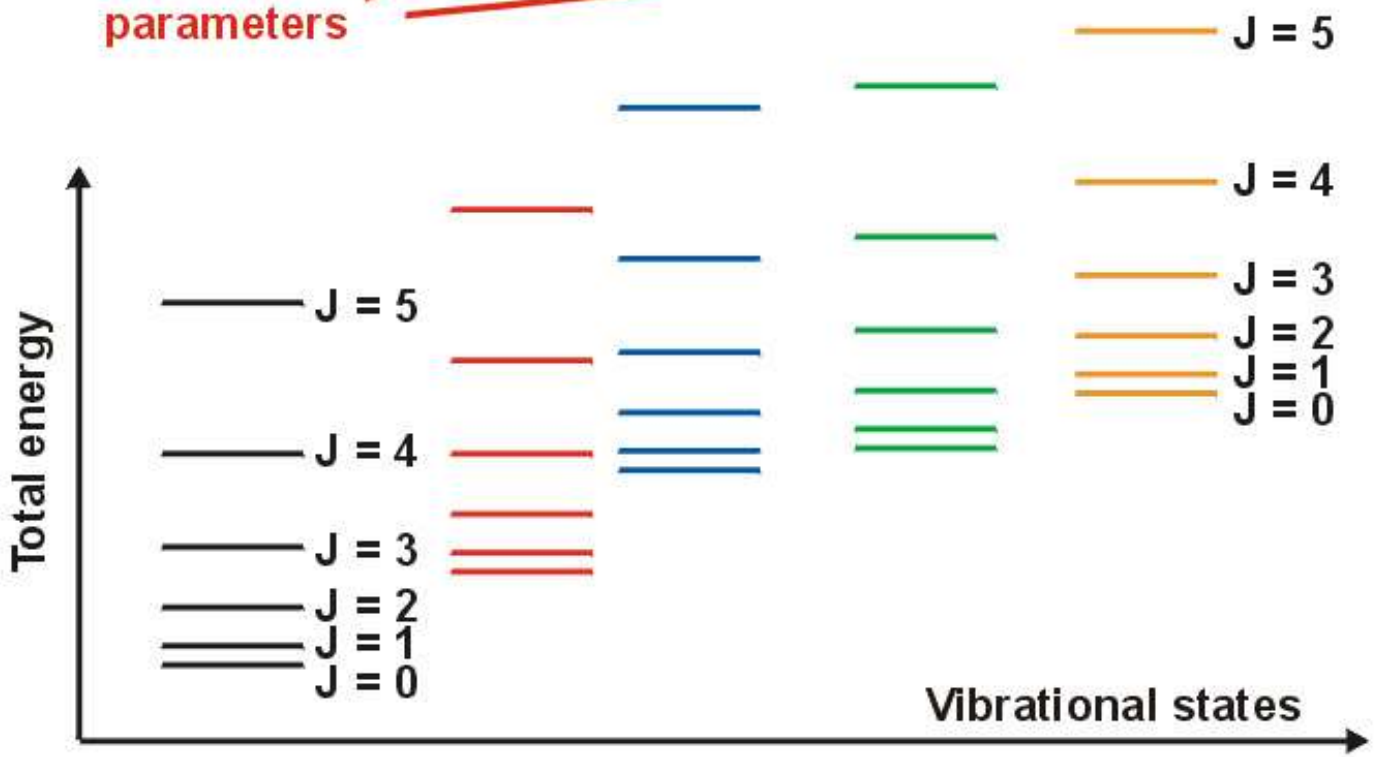
$$E = E_{vib} + B\left[J\left(J+1\right) - k^2\right] - D\left[J\left(J+1\right) - k^2\right]^2$$

Vibrational energy

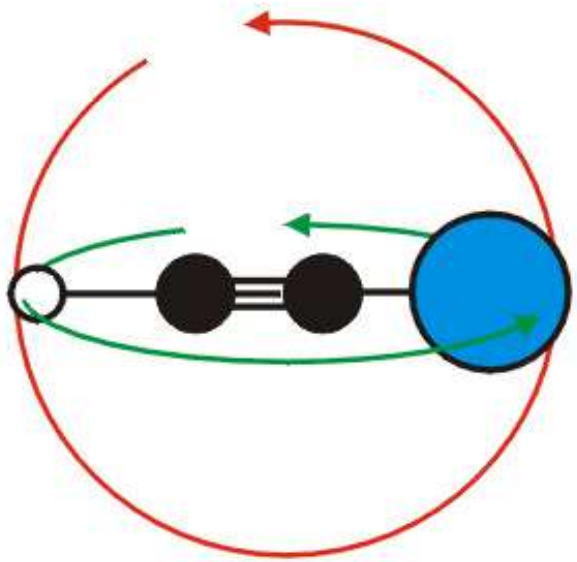
Rigid rotor energy

Centrifugal distortion

Structure parameters



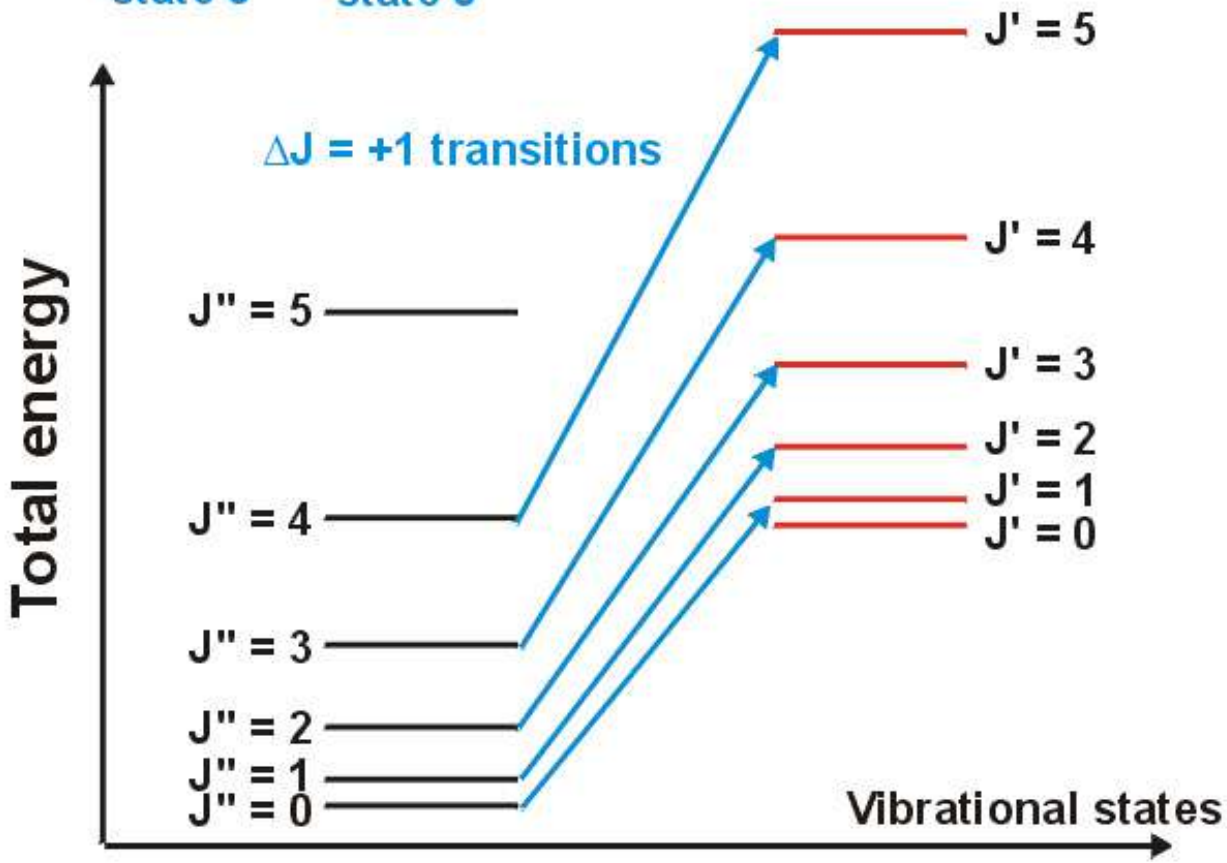
Rotation is degenerate around x- and y-axis



Transitions

Selection rule $J' = J'' \pm 1$

Upper state J — Lower state J

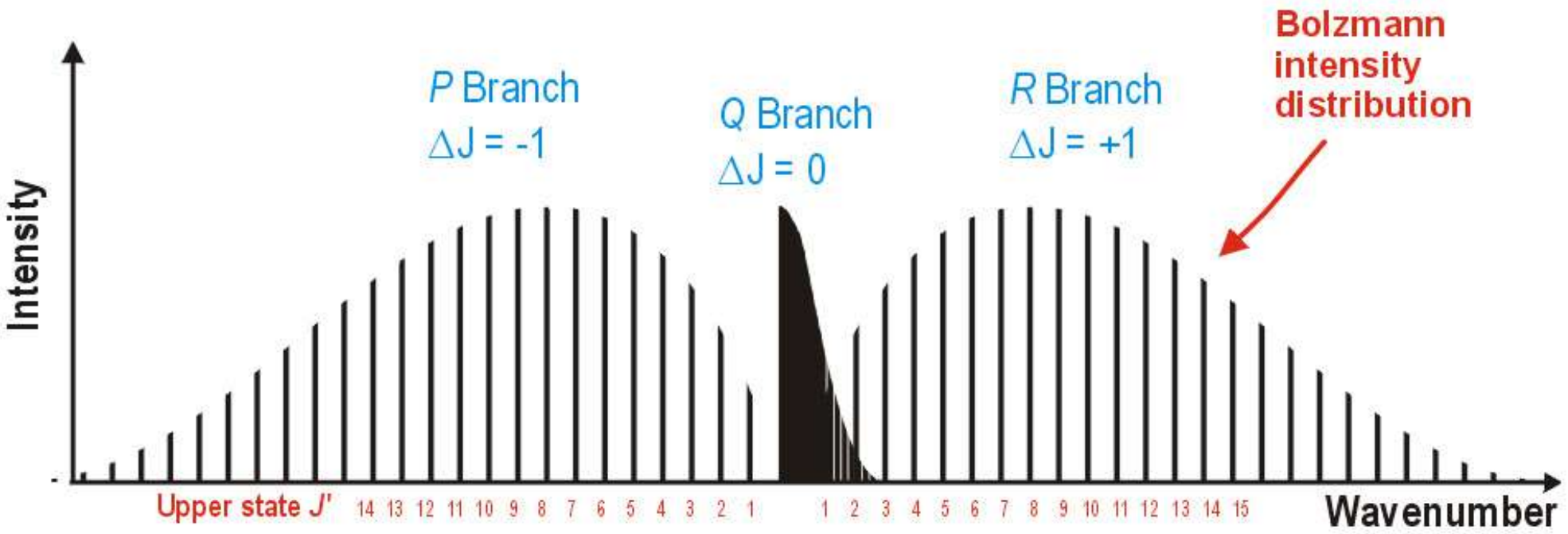


Transition energy $\tilde{\nu} \simeq \Delta E_{vib} + 2BJ' + \cdots$

Vibrational transition — Rotational transition

Spectrum bands

Transition energy $\tilde{\nu}_R \cong \Delta G_v + 2BJ' + \ldots$



Band systems

Several overlapping bands form a band system

Ground state: high population & intensity

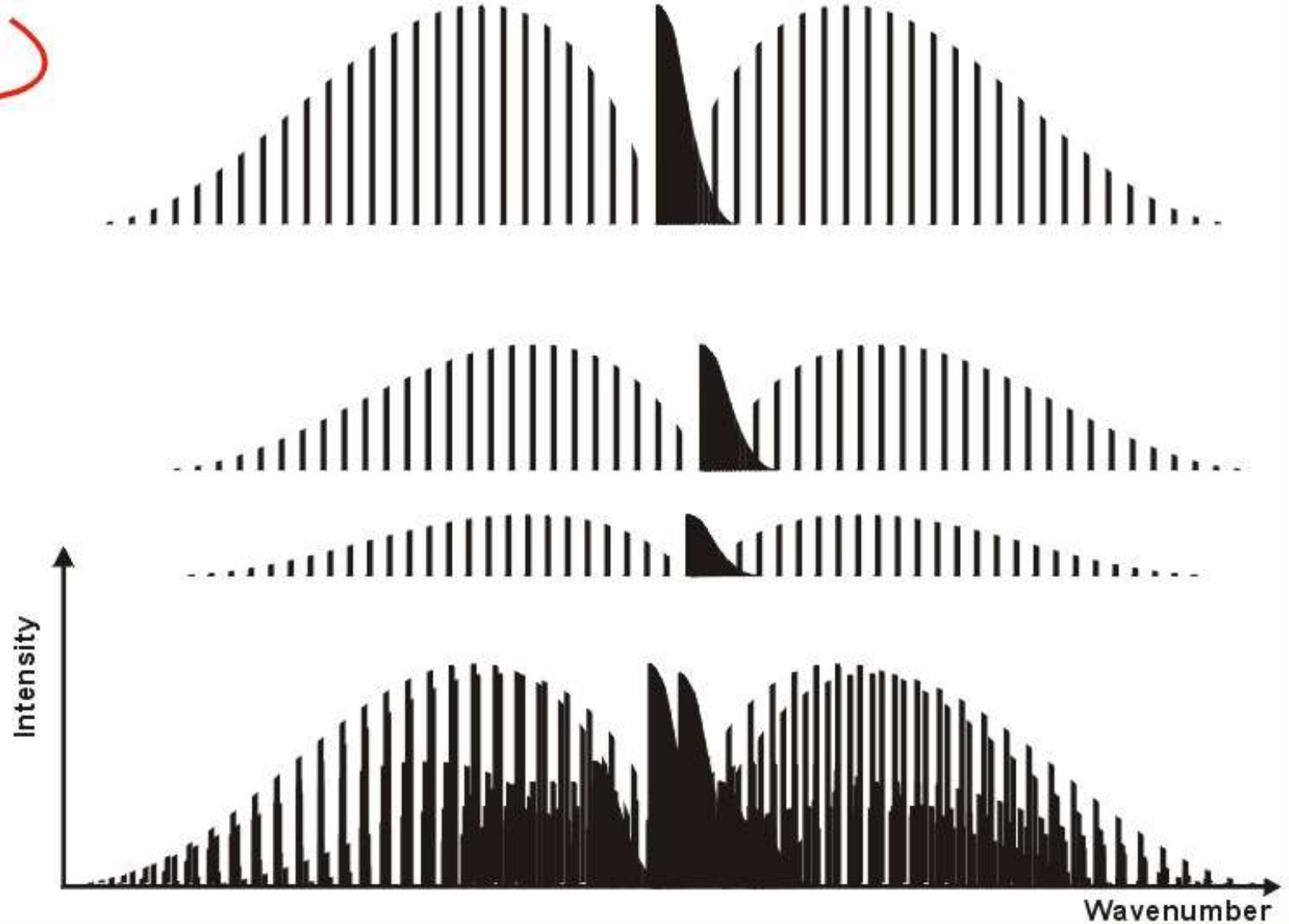
$|0,1,1\rangle \leftarrow |0,0,0\rangle$

Upper vib.state **Lower vib.state**

Excited states: low population & intensity

$|0,1,2\rangle \leftarrow |0,0,1\rangle$

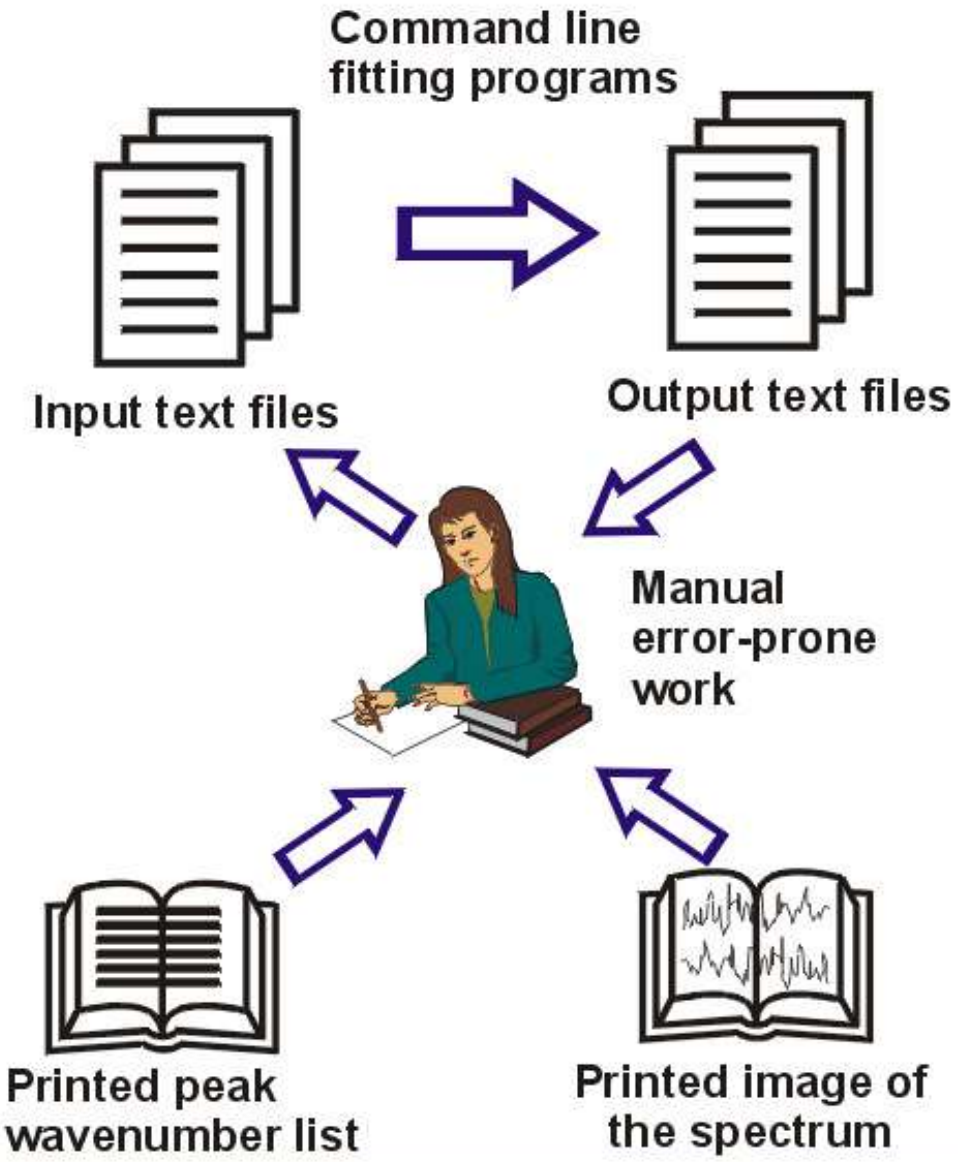
$|0,2,2\rangle \leftarrow |0,1,1\rangle$



Observed Spectrum

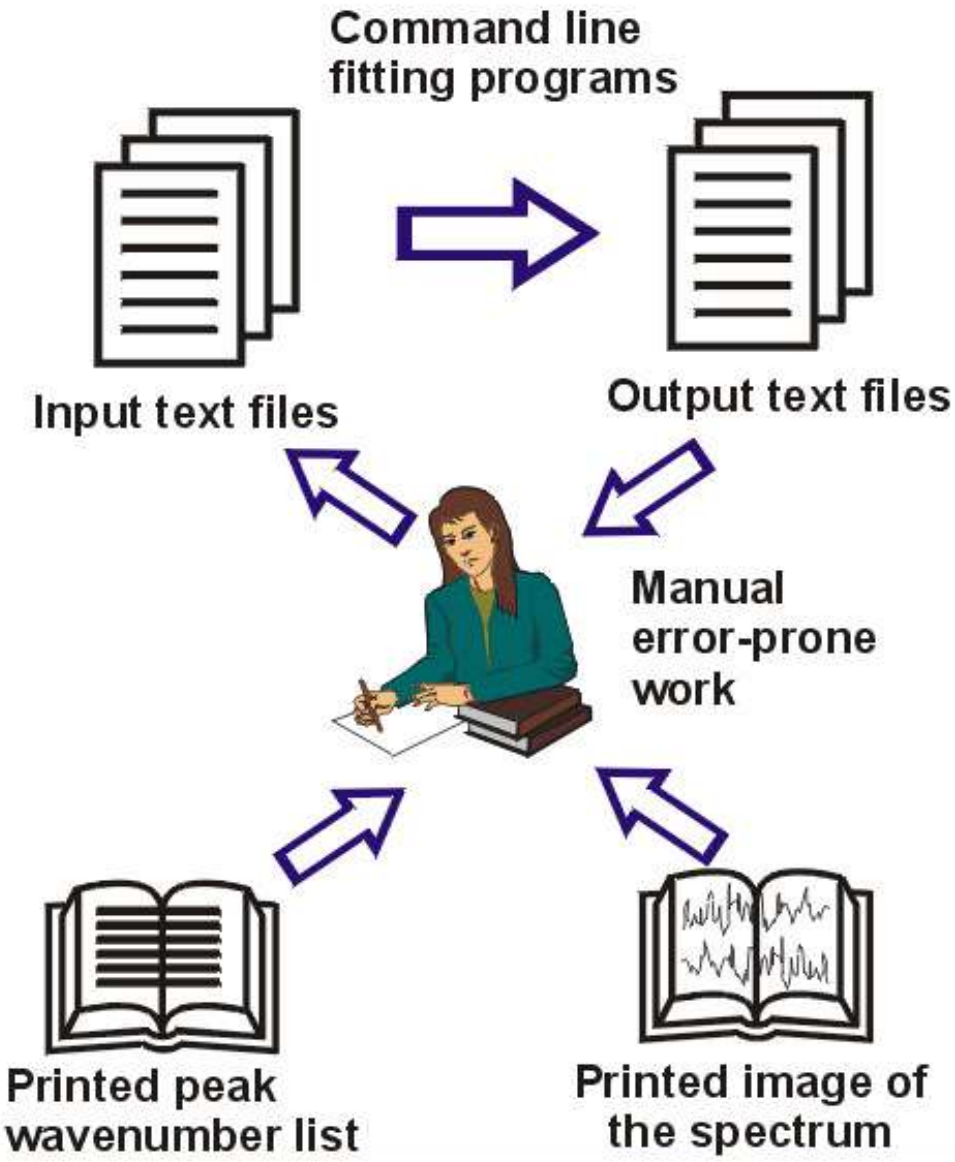
Infia vs. Traditional analysis tools

Traditional tools:
Nonvisual, manual

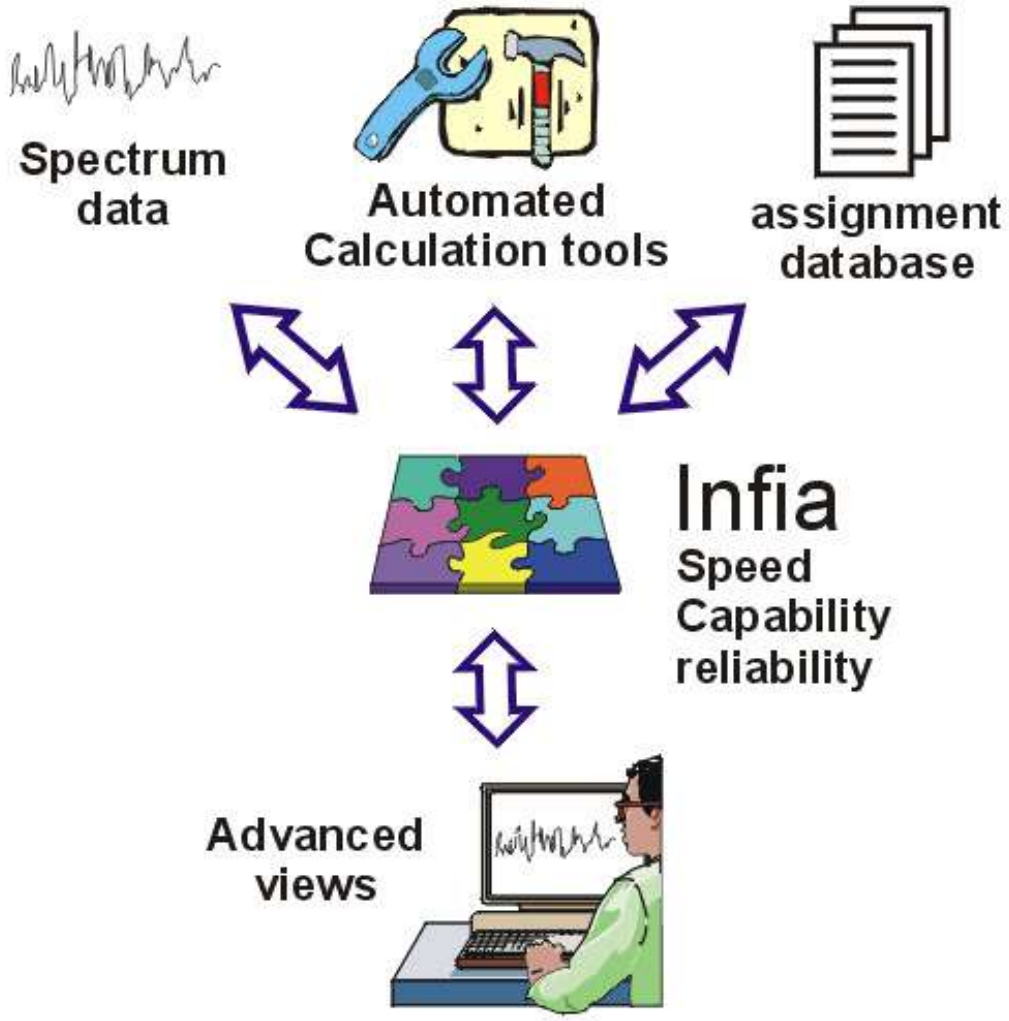


Infia vs. Traditional analysis tools

Traditional tools: Nonvisual, manual



Infia: Visual, interactive, automatic



Branch combination

Assigment problems

- How to extend the assignments of a band from the P branch to the R banch (or vice versa)?
- How to determine the correct vibrational lower state of a hot band?
- How to determine the correct J assignments?

Solution

Combination Difference Prediction

Repeat:

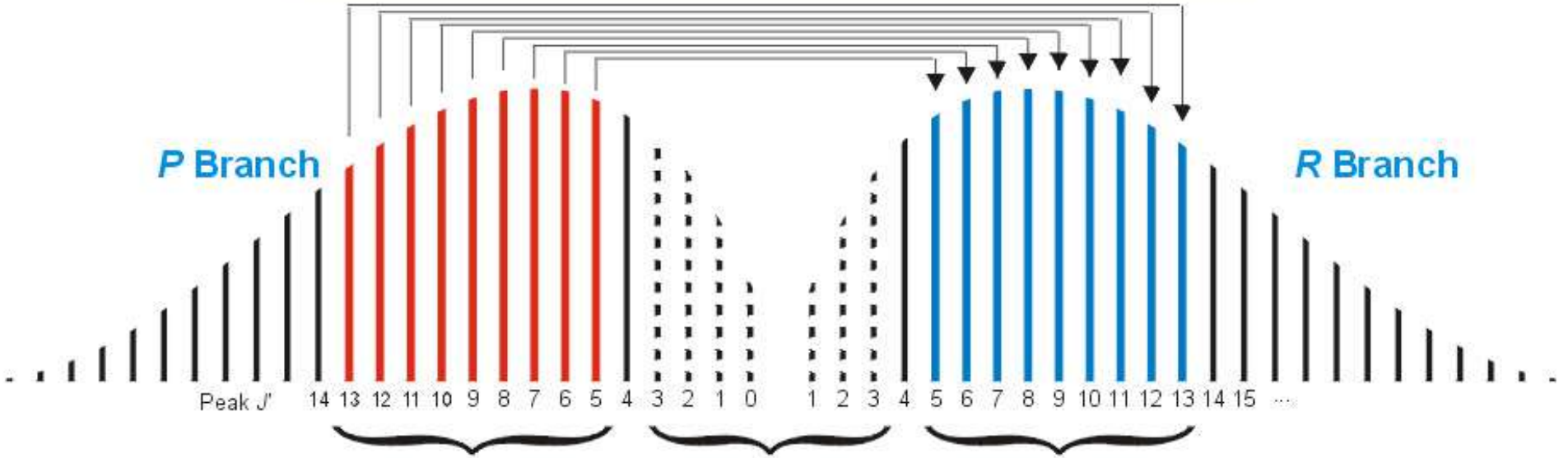
- Guess lower state
- Guess shift in m assignments
- Calculate predictions in R branch with *combination difference* formula
- Evaluate the predictions againts spectrum lines using *Fitness* function

Until good lower state / m combination found

Branch combination

$$\tilde{\nu}_r = \tilde{\nu}_p + (4B'' - 6D'')(J' + \tfrac{1}{2}) - 8D''(J' + \tfrac{1}{2})^3$$

Combination difference formula



Selection of the correct band assigment

Branch combination results

- Complete band with *P* and *R* branches.
- Correct lower state
- Correct *m* assignments

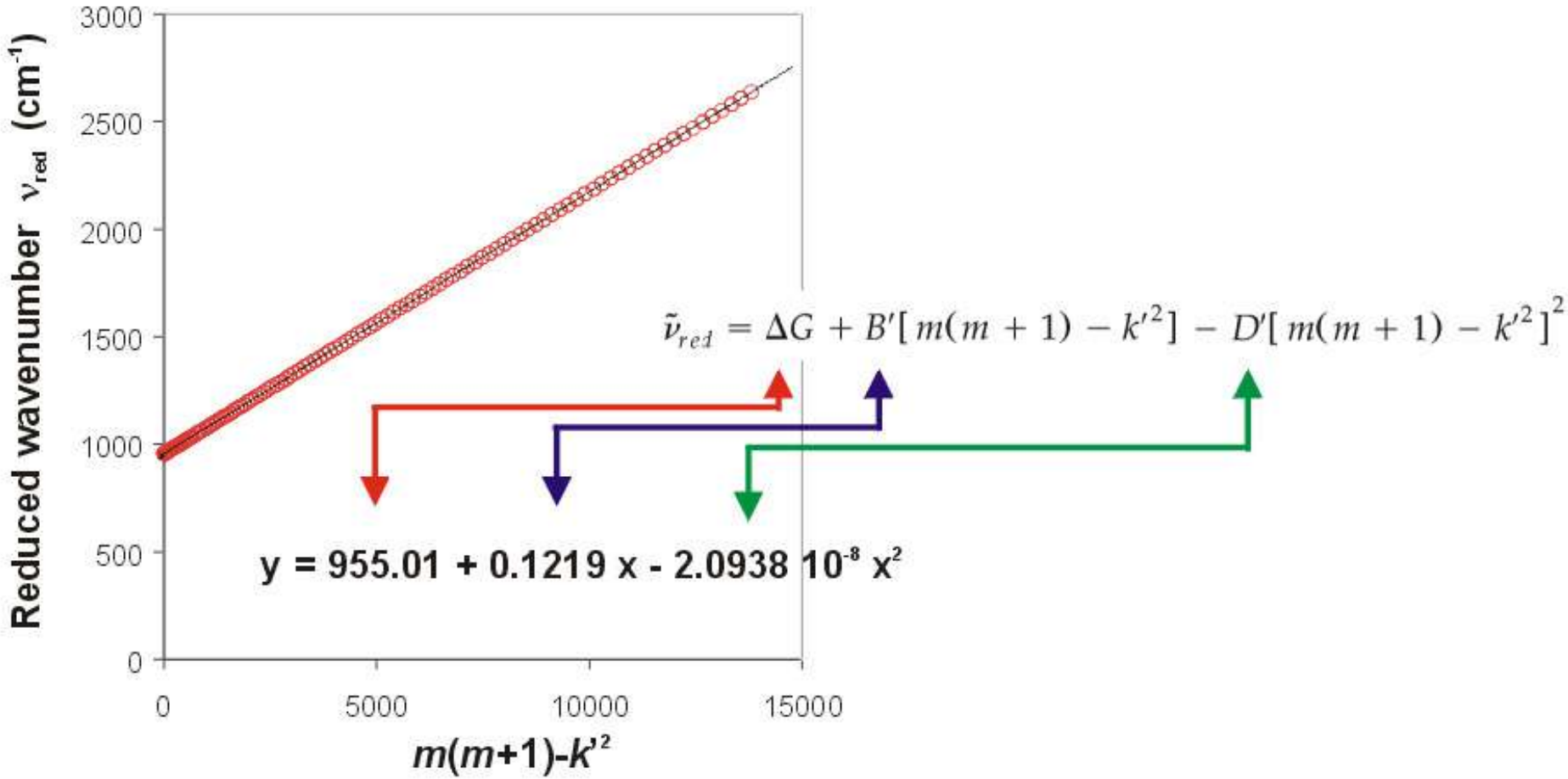
Parameter calculation

Aim: Accurate determination of upper vibrational state parameters (B, D,...)

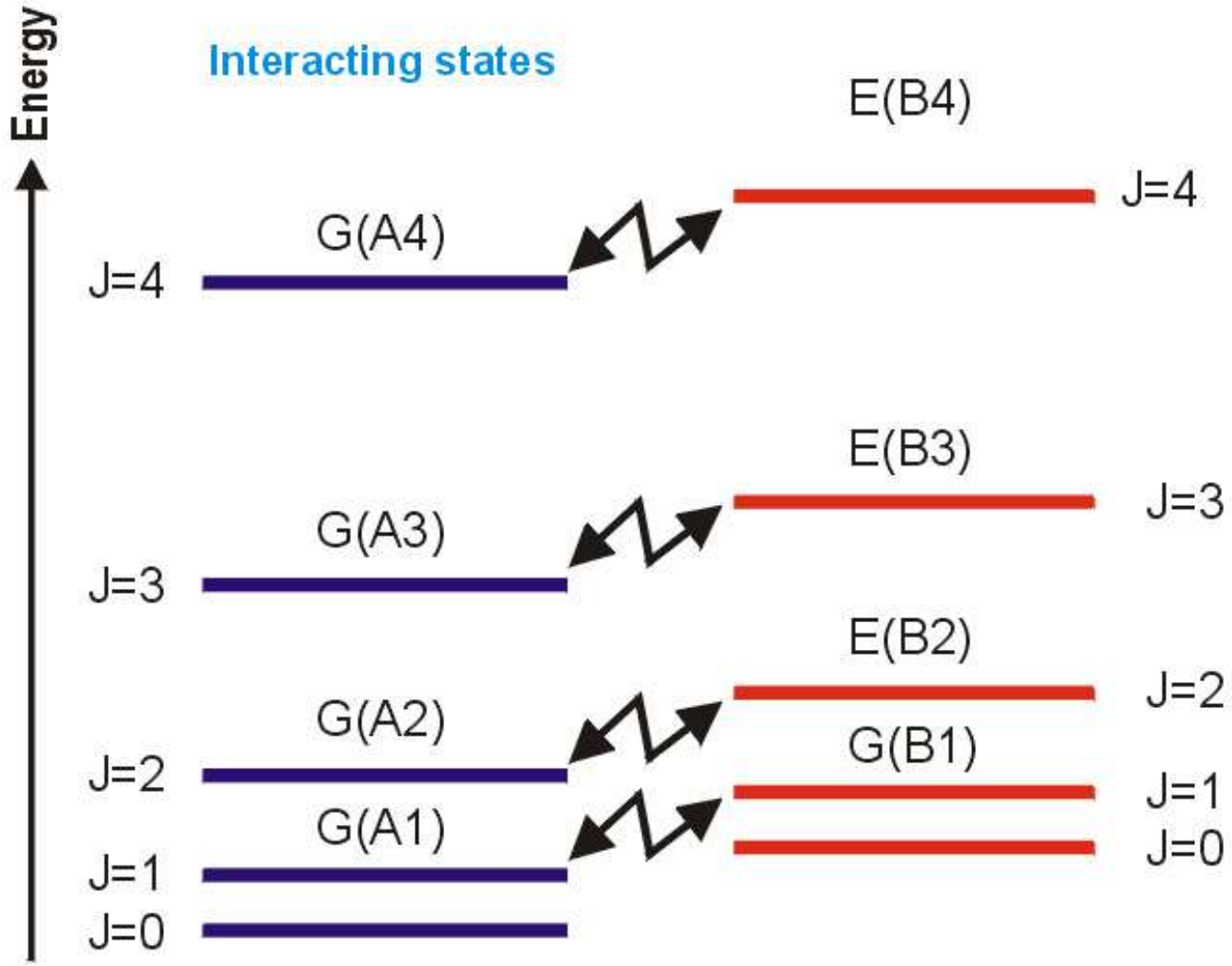
Solution: Substract known lower state energies from transitions and perform a polynomial fit for upper state parameters

Reduced wavenumbers

$$\tilde{\nu}_{red} = \Delta G + B'[\,m(m+1) - k'^2\,] - D'[\,m(m+1) - k'^2\,]^2$$



Resonance calculations



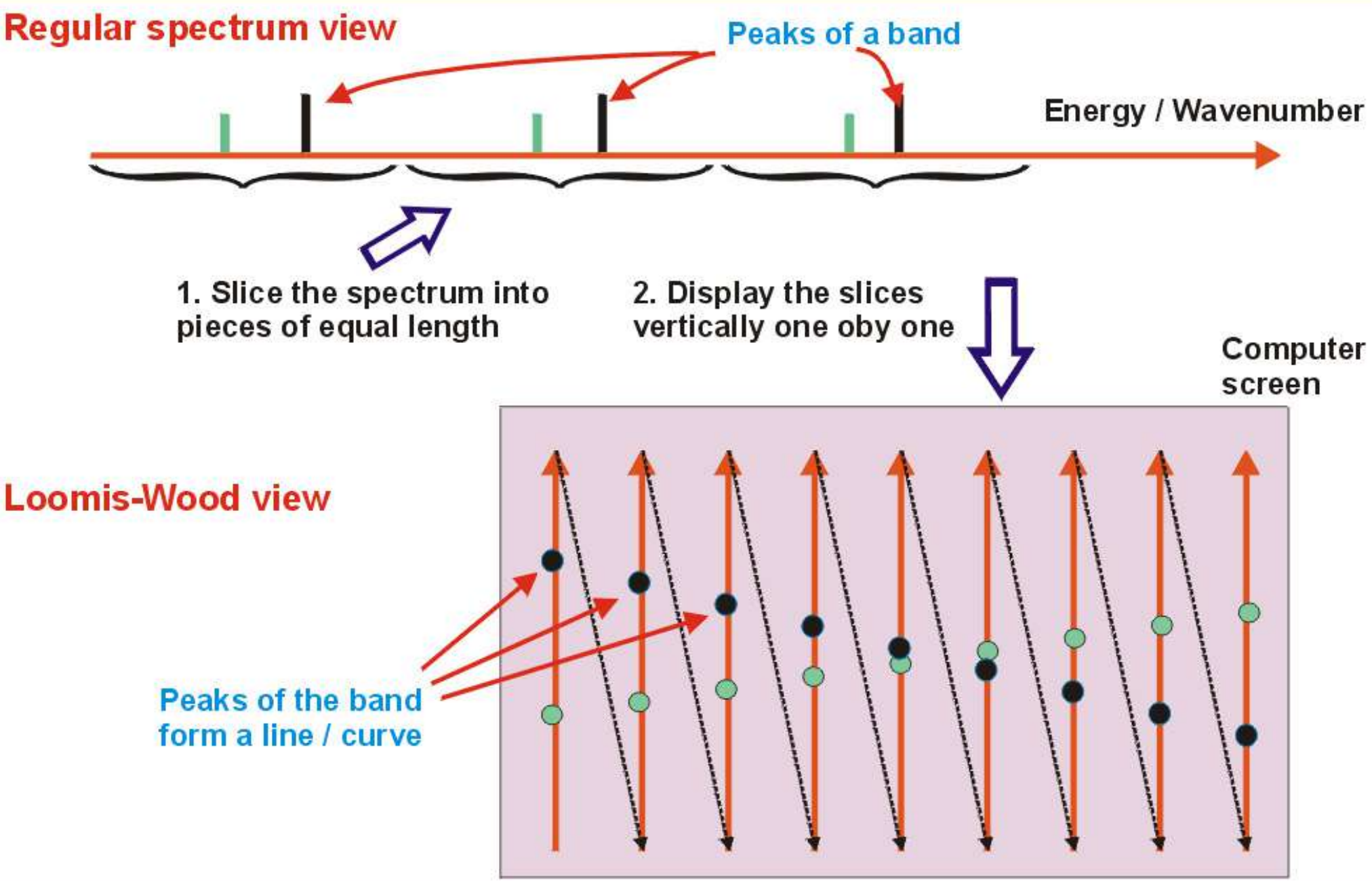
Off-diagonal resonance matrix elements perturb vibration-rotation states

Hamilton matrix diagonalisation

	A	B
A	G_A	$f_L(q_t,J)$
B	$f_L(q_t,J)$	G_B

Non-linear least squares optimisation

Loomis-Wood view



Summary

Features

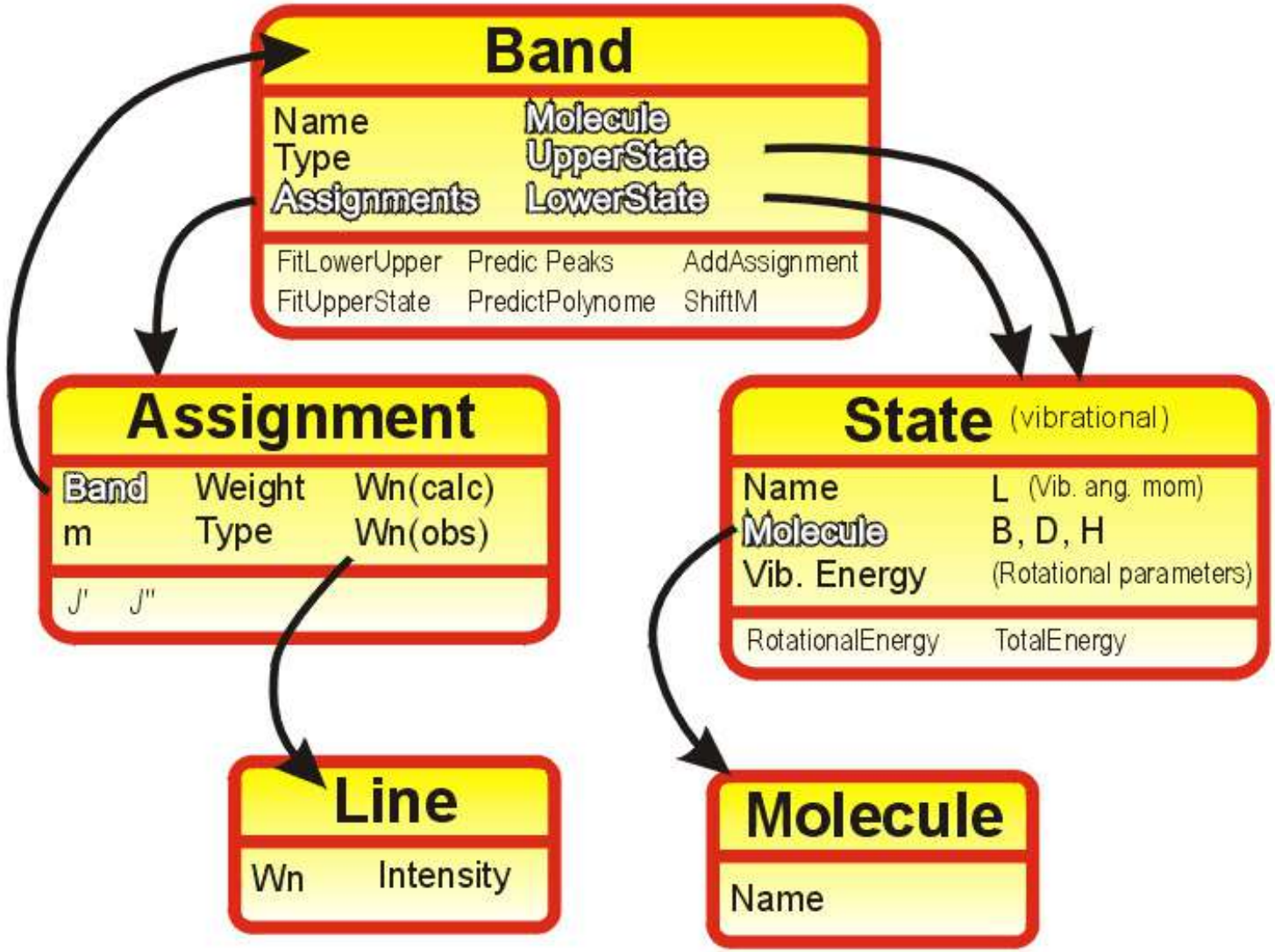
- Advanced interactive views
- Integrated assignment database
- Integrated calculation tools
- Automatic comb difference prediction

Advantiges

- Rapid spectrum analysis
- Avoiding of human typing errors
- Finding more spectrum features

Infia program design

* Object oriented programming
* Delphi 4
* 32bit Windows development
* 5000 lines of code
* Extensible design



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