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Renaissance in diatomic spectroscopy

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quest

Molecule AB

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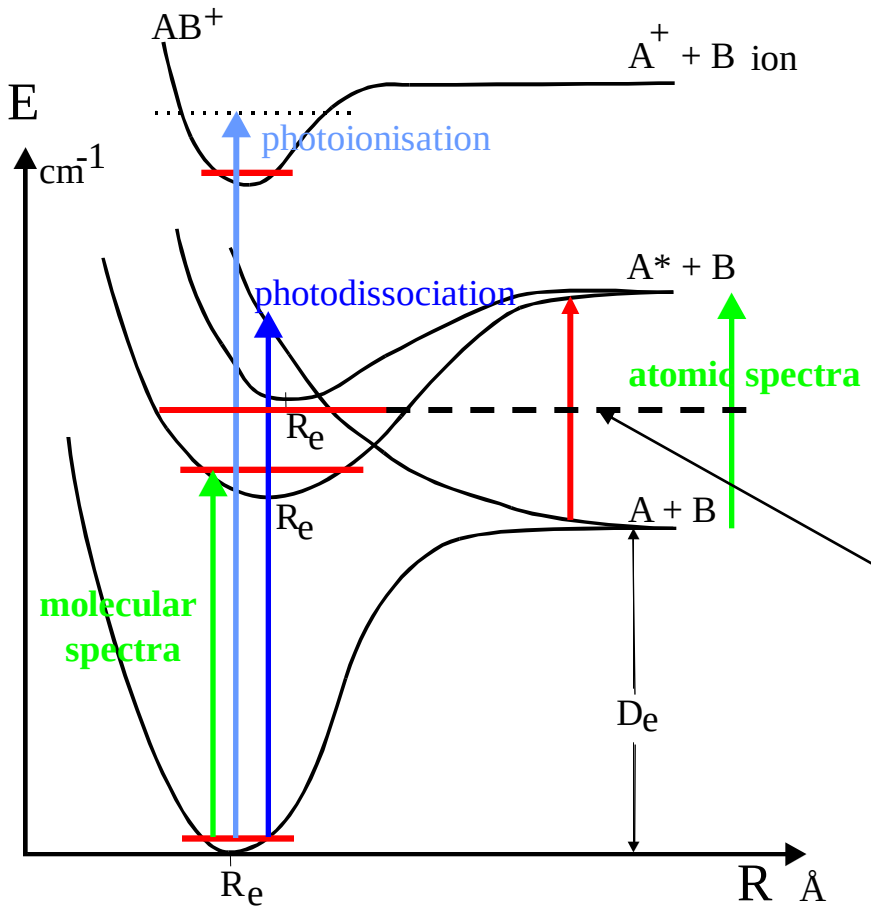

molecular spectra

quantum numbers, configuration, potentials

photodissociation, "half" collision

photoionisation, photoelectrons, ZEKE, autoionisation **ionisation energy**

potential crossing, coupling of states
predissociation
Feshbach resonance

$A + B + h\nu \rightarrow AB^*$ **photoassociation**

$A + B \rightarrow A' + B'$ collisions, collisions in fields, optical collisions, etc.

Band spectra and requirements on resolution

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- classical spectroscopy:
  - diffuse bands
  - band heads and vibrational systematic
  - shaded bands and rotational energy
  - molecular parameters
    - Herzberg: ω_e, $\omega_e x_e$, … B_e, α_e, …
    - Dunham: power series in v+1/2 and J(J+1) Y_{kl}
  - compact form of large data sets of rovibrational structure
- microwave spectroscopy:
  - rotational energies, hyperfine structure, Stark- and Zeeman effect
- laser spectroscopy:
  - high resolution, Doppler reduced, non-linear methods etc.
  - looking with a magnifying glass
- Fourier transform spectroscopy

varying the application of light

- Ultracold matter as new kind of ensemble

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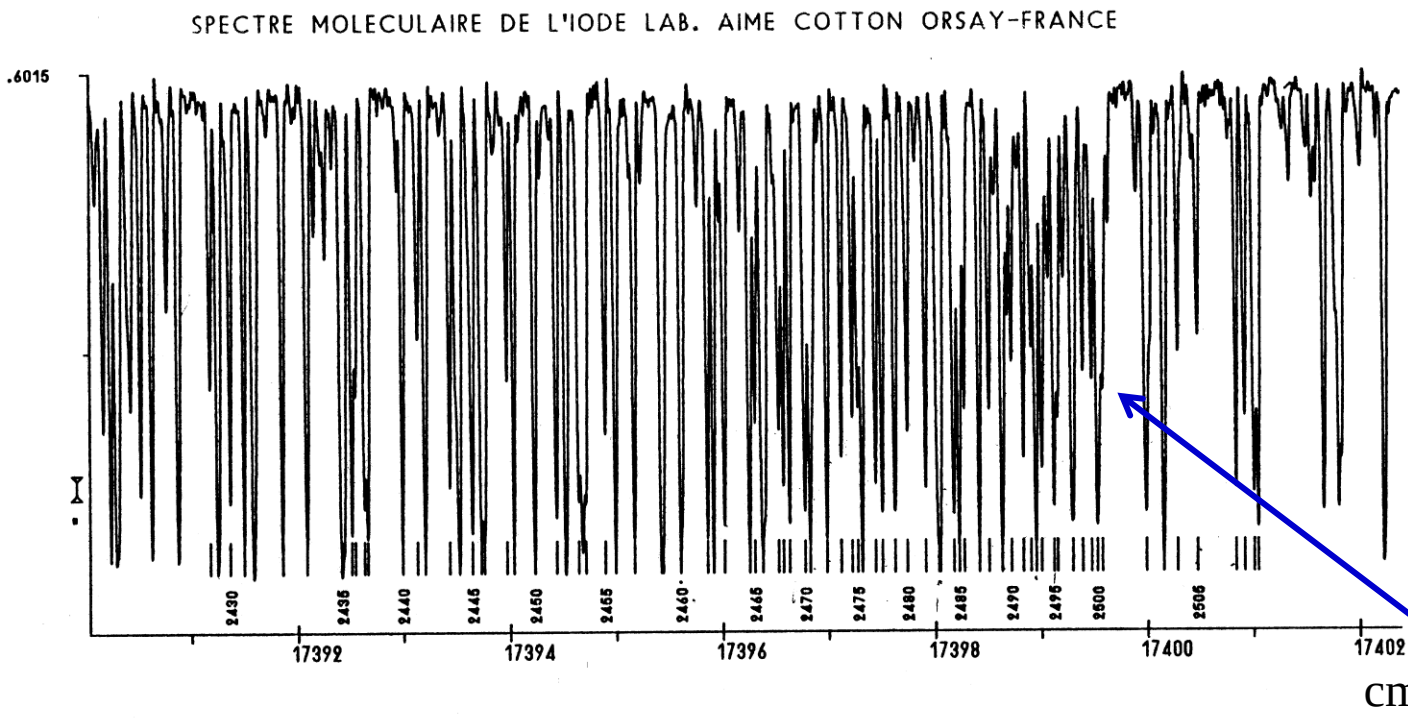
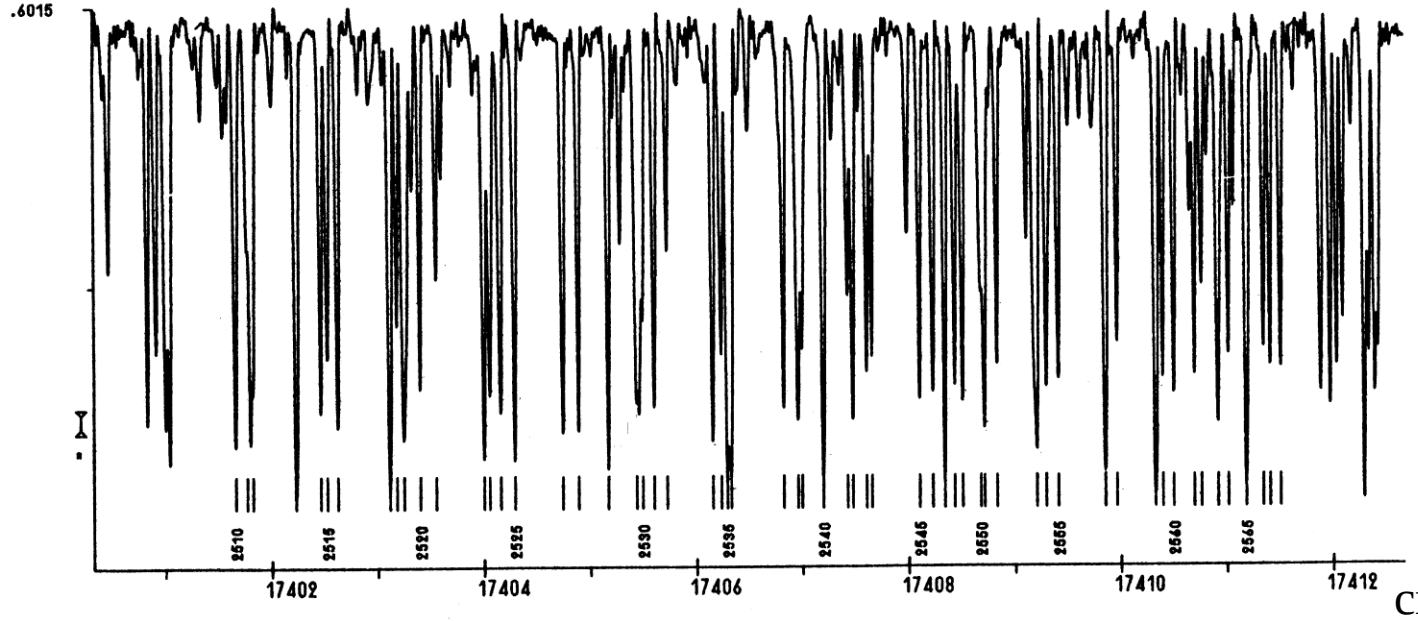
Some remarks to the state of the art in conventional spectroscopy





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High resolution absorption spectra by Fourier spectroscopy

resolution 0.01cm^{-1}
accuracy 0.003cm^{-1}

dense!

Iodine atlas
Gerstenkorn/Luc
Orsay

Synthetic band spectra

example I_2 T = 900K

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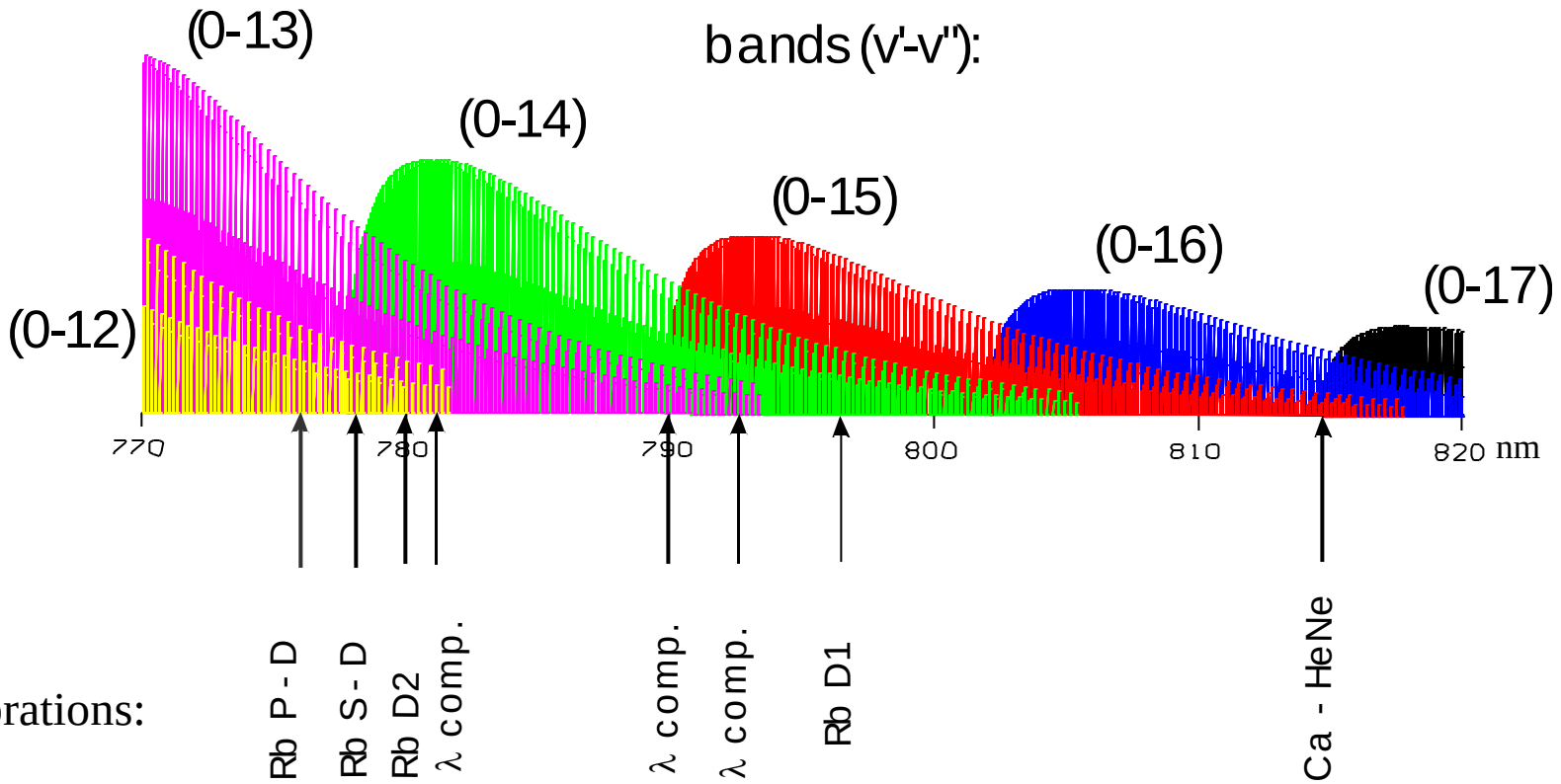

Spectra simulation of optical spectrum of Iodine

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iodine atlas on the notebook
poor man's secondary frequency standard

accuracy: in general 0.003cm-1 or 100MHz
areas better than 10 MHz and some better than 1MHz
$\Delta\nu/\nu$ up to 10^{-9}

reproducibility: depends on the preparation of the absorption cell
pressure shift, temperature dependence

www.iqo.uni-hannover.de
→ Molecules & Lasers → Secondary Frequency Standard

What is behind such simulation?

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huge data set of high precision from several sources

← checked internal consistency!

assignment of spectra

model Hamiltonian:

molecular potentials replace molecular parameters

or

coupled system with potential matrix → “deperturbation”

fitting procedure → compact form of “all” data

by potentials and simple coupling functions

New era
“ultracold matter and molecular spectroscopy”

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dense ultracold ensemble of atoms

start with pure atomic ensemble
only one or two quantum states

interaction: light and/or collisions

design a quantum specific pathway
to molecules

ensemble with atoms and molecules
statistical distribution?

spectroscopy can and will provide
the data about the interactions

new chances

design the ensemble with reduced dimensionality or spatially ordered

↓ cigar or disk shape

↓ optical lattice

Different experimental situations!

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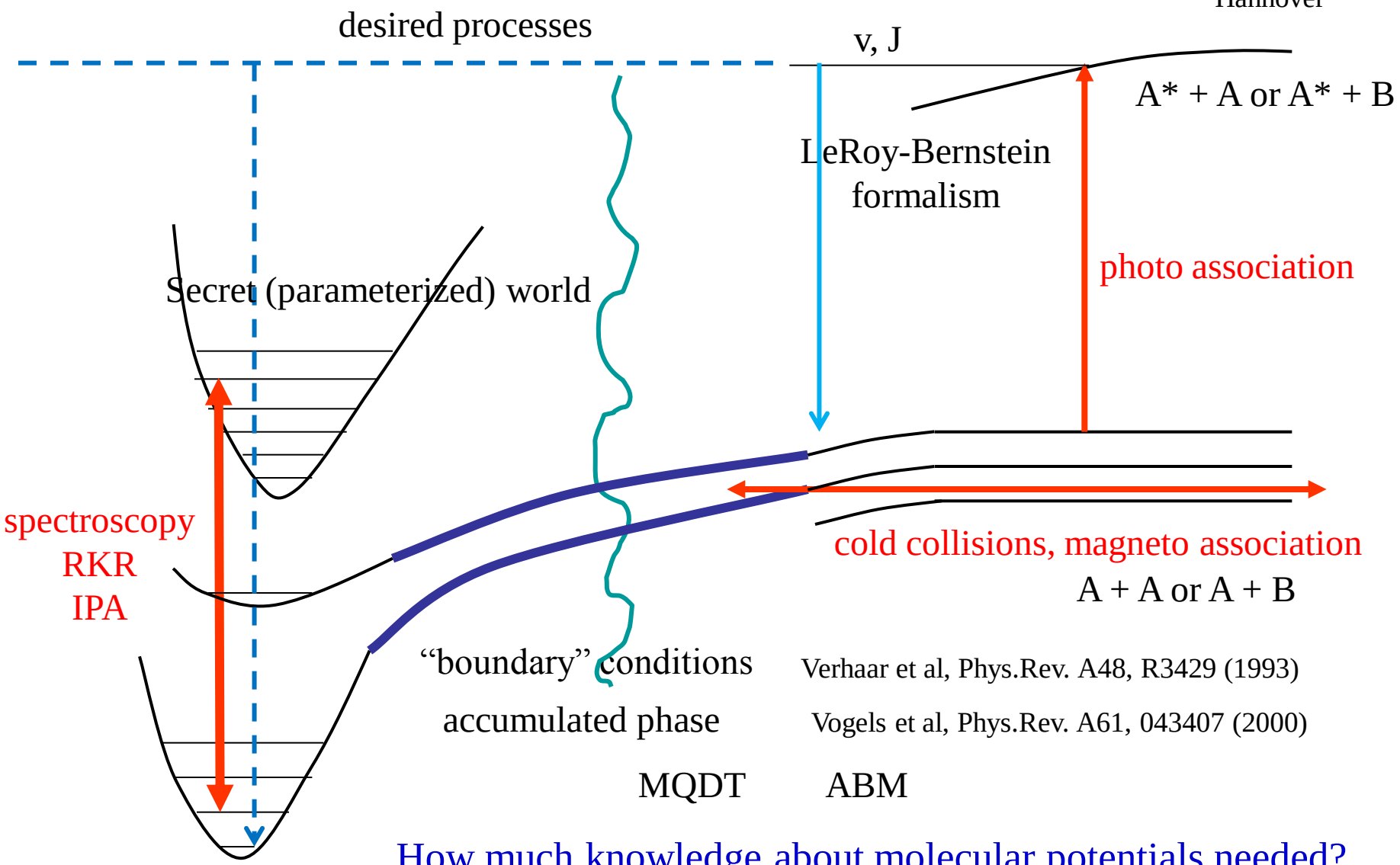

Verhaar et al, Phys.Rev. A48, R3429 (1993)

Vogels et al, Phys.Rev. A61, 043407 (2000)

How much knowledge about molecular potentials needed?

The spectroscopic workhorse

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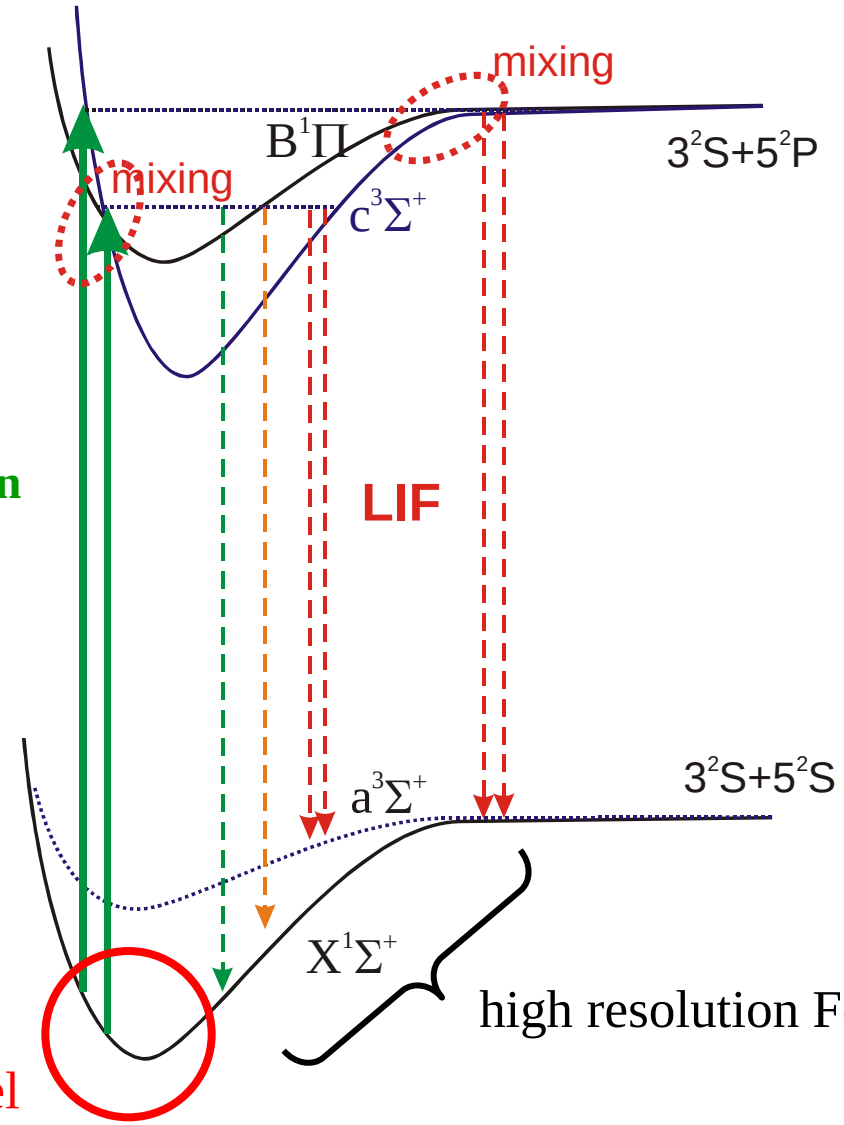

Laser excitation

LIF

high resolution Fourier spectroscopy

entrance channel

Example NaRb

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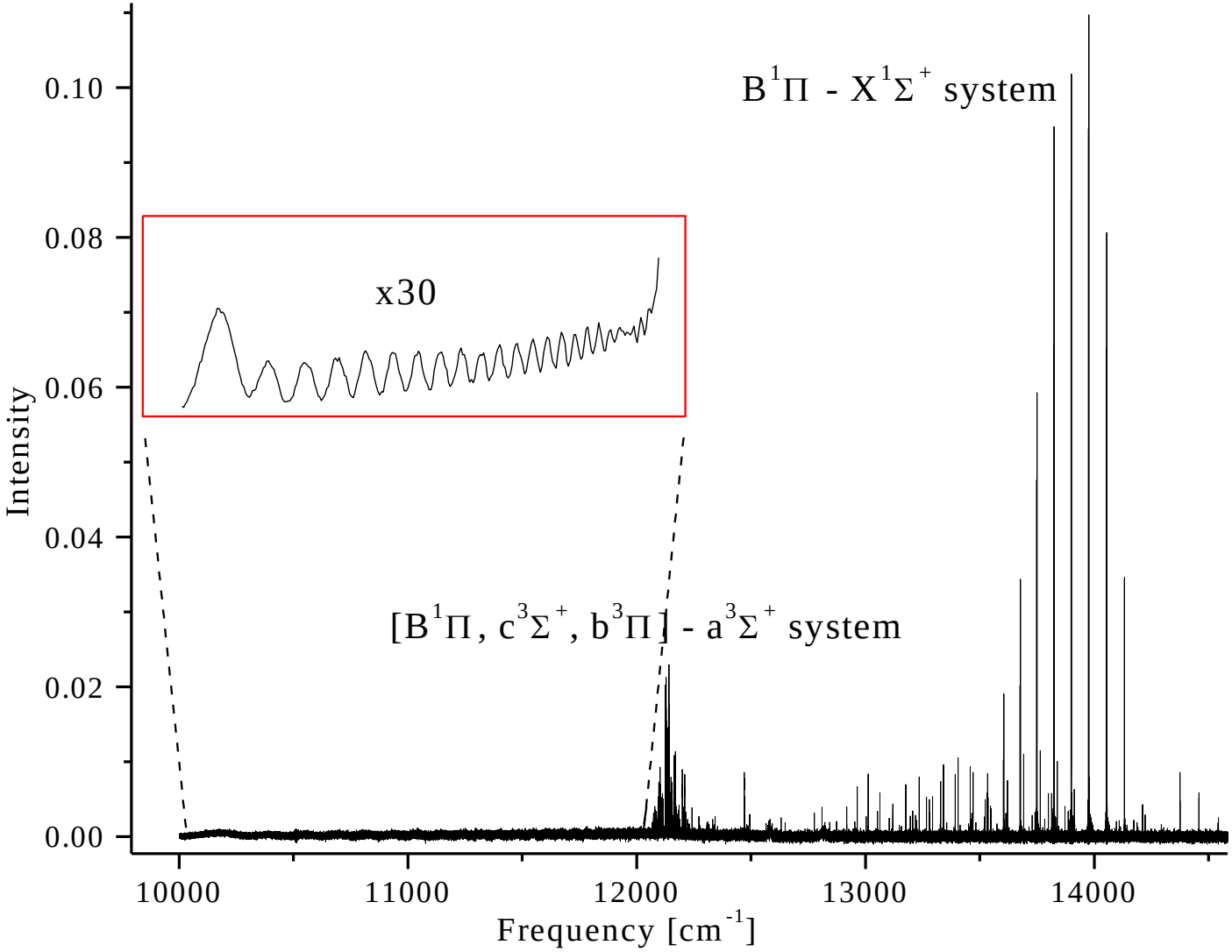

Example Sr_2 with a large data

application of molecular data → atomic clock with Sr

Set of molecular levels for Sr_2

area of possible levels

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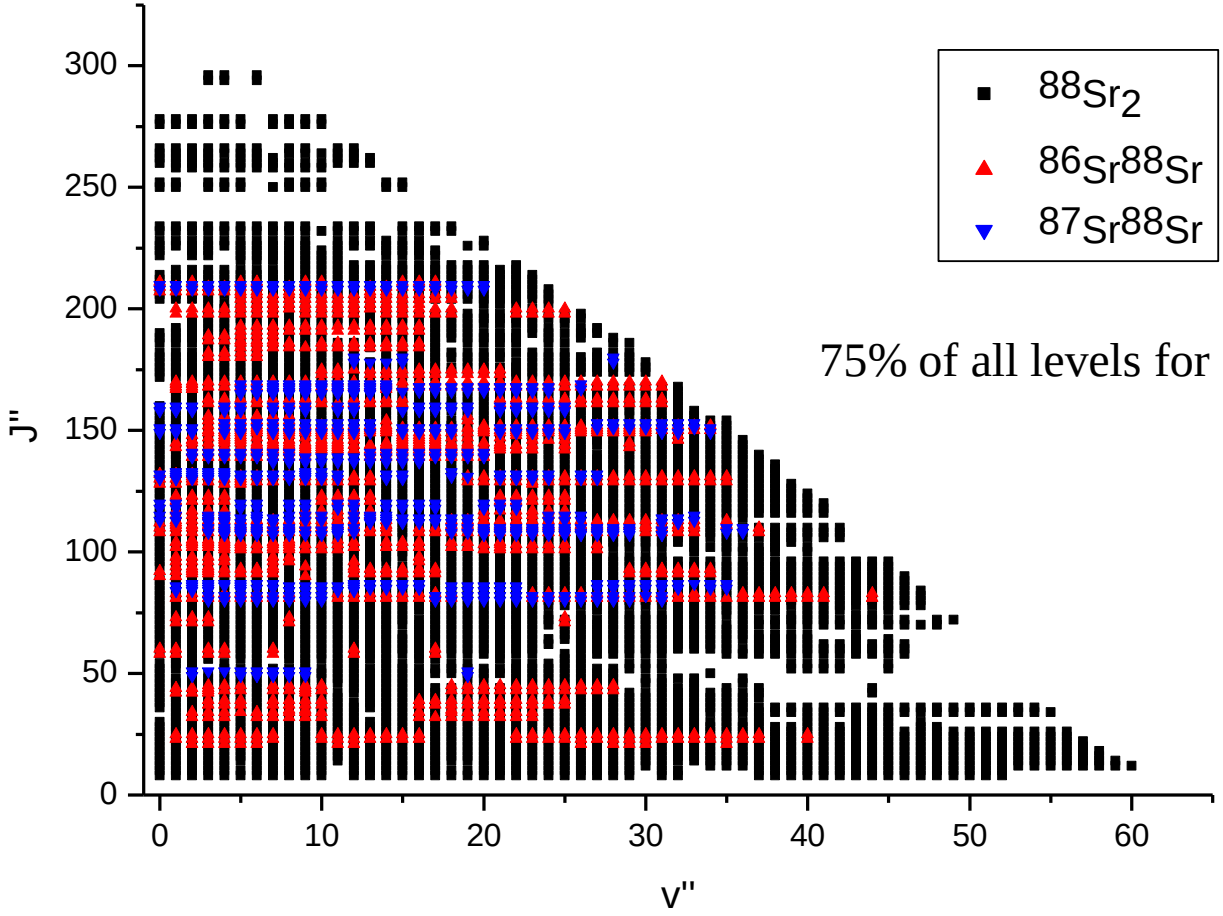

75% of all levels for $^{88}Sr_2$ observed

Derive a continuous function for the potential?!

Yes with 23 free parameters for 6077 data points

Ground state of Sr_2

Eur. Phys. J. D **57**, 171–177 (2010)

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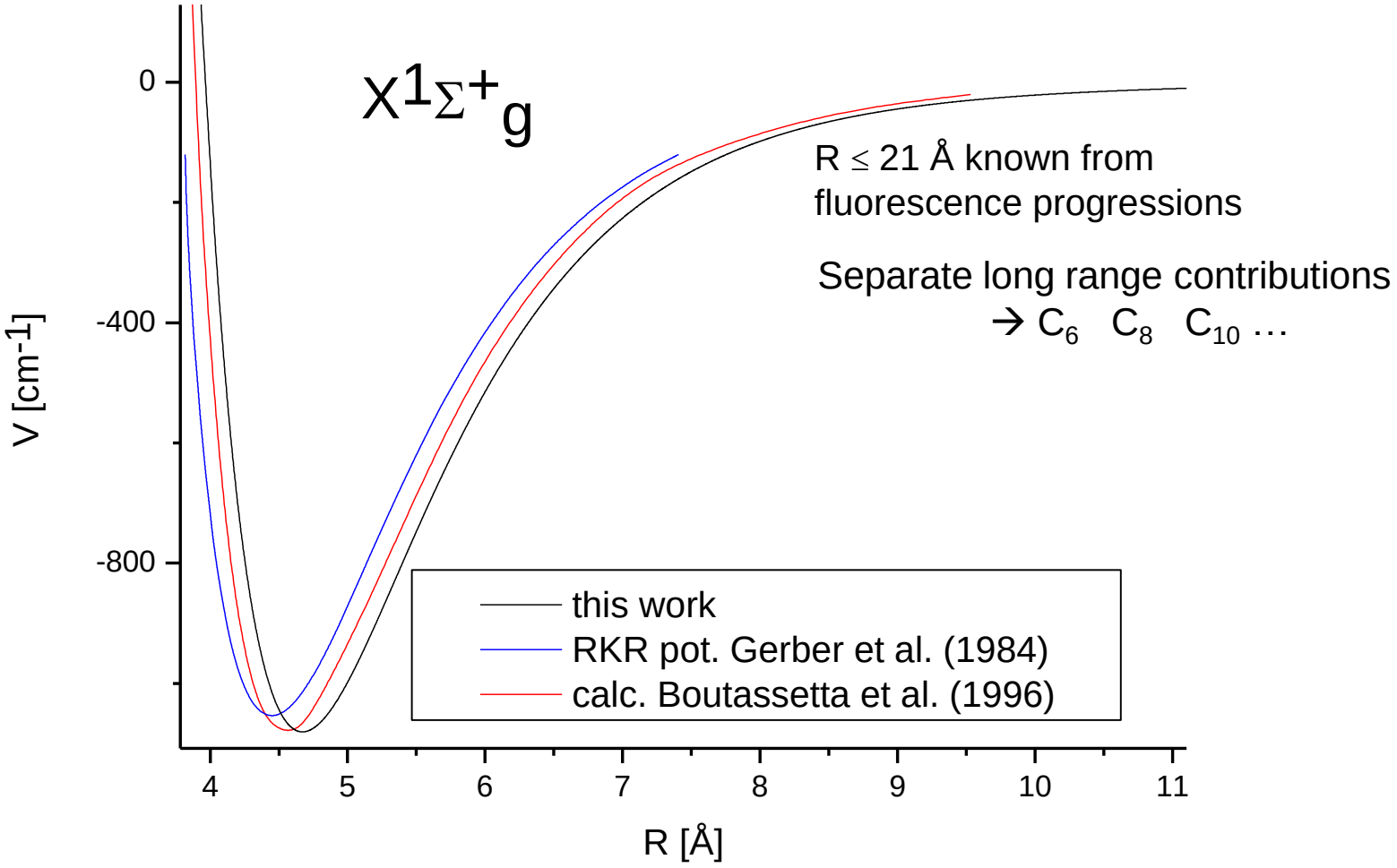

How precise are experimentally derived potentials?

Excitation scheme for pair spectroscopy

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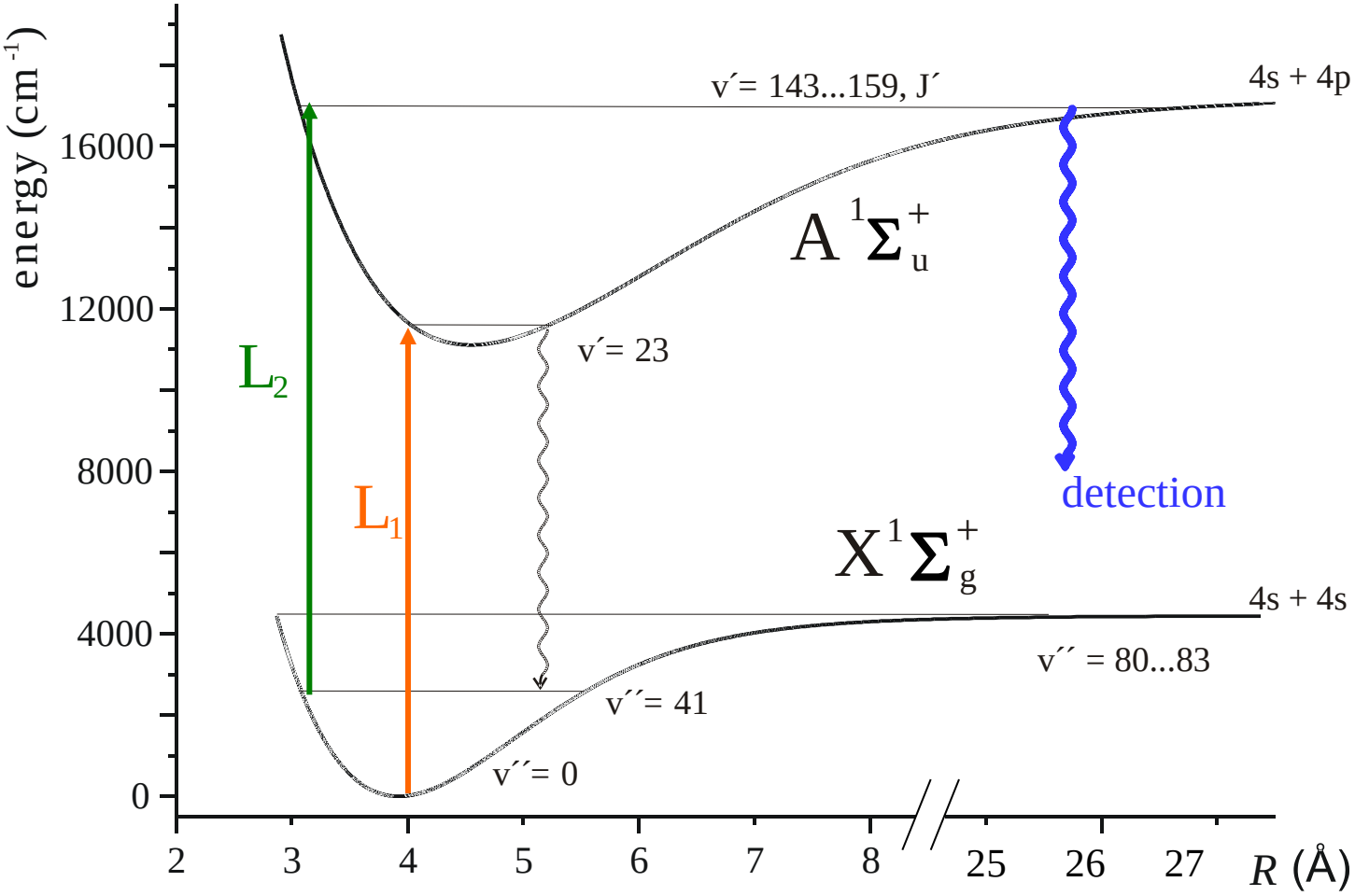

Preparing atom pairs

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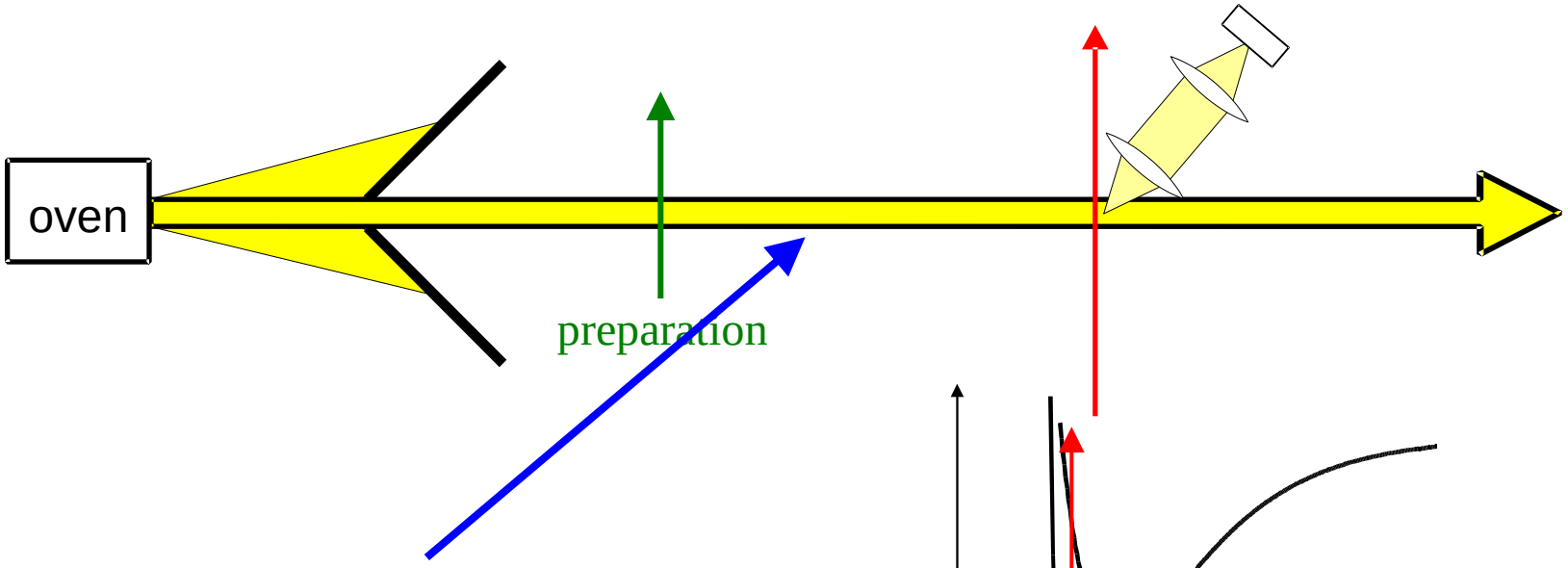
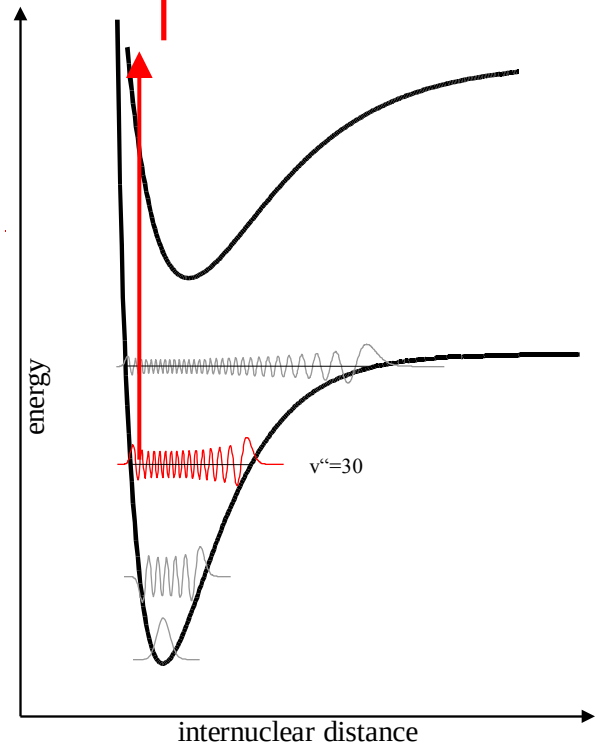


high v“ populated

asymptotic vibrational levels become observable



Atom pairs in K_2 beam

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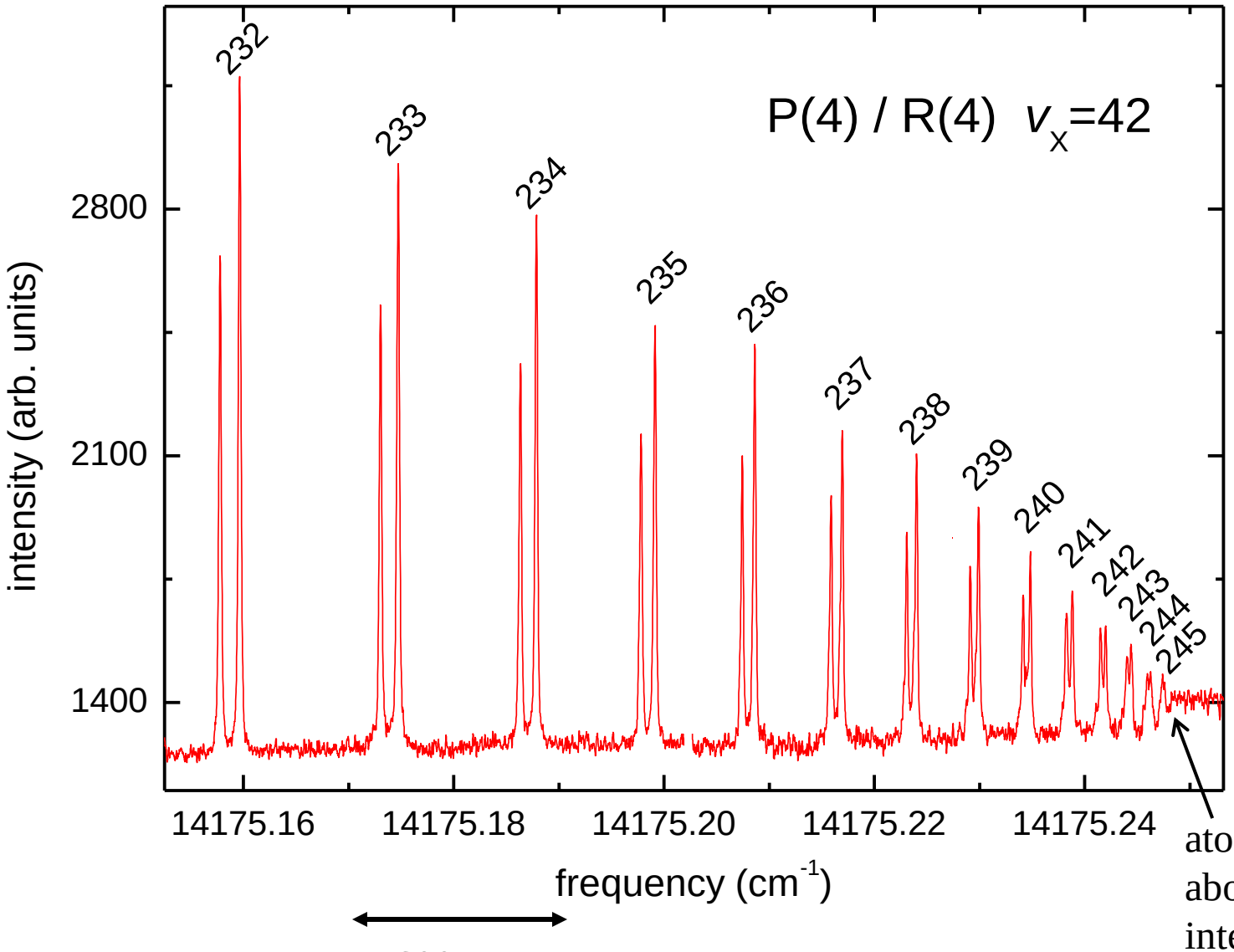

dissociation!

atom pair
about 300 Å
internuclear separation

Coherent excitation scheme to the cold collision regime

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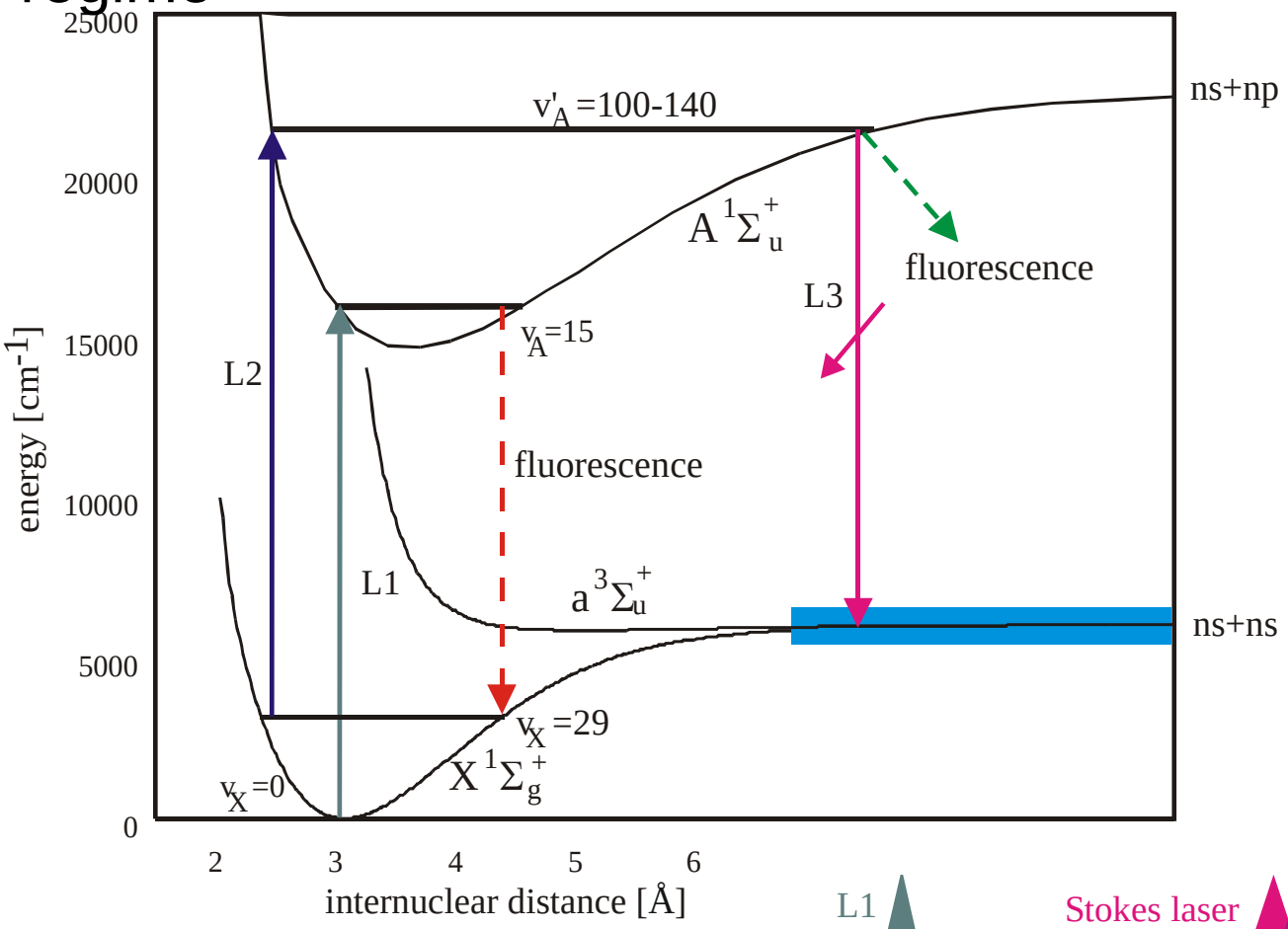
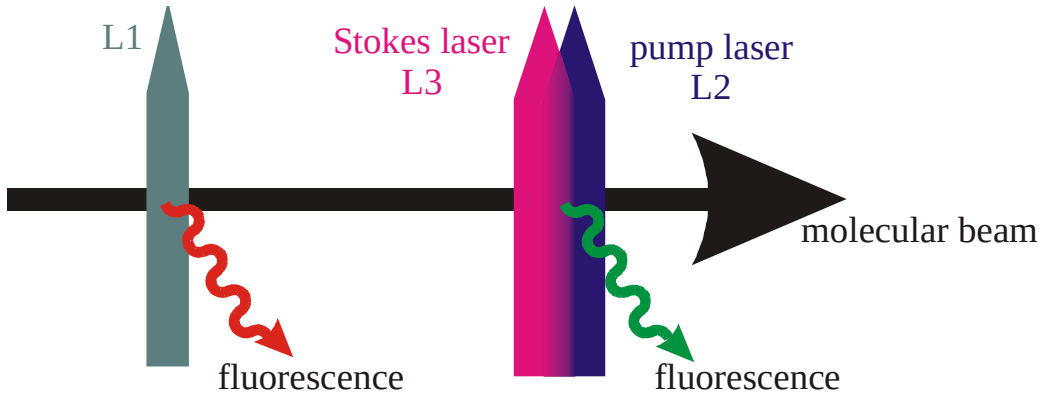


Example Na_2



Scattering spectroscopy → inverted photoassociation

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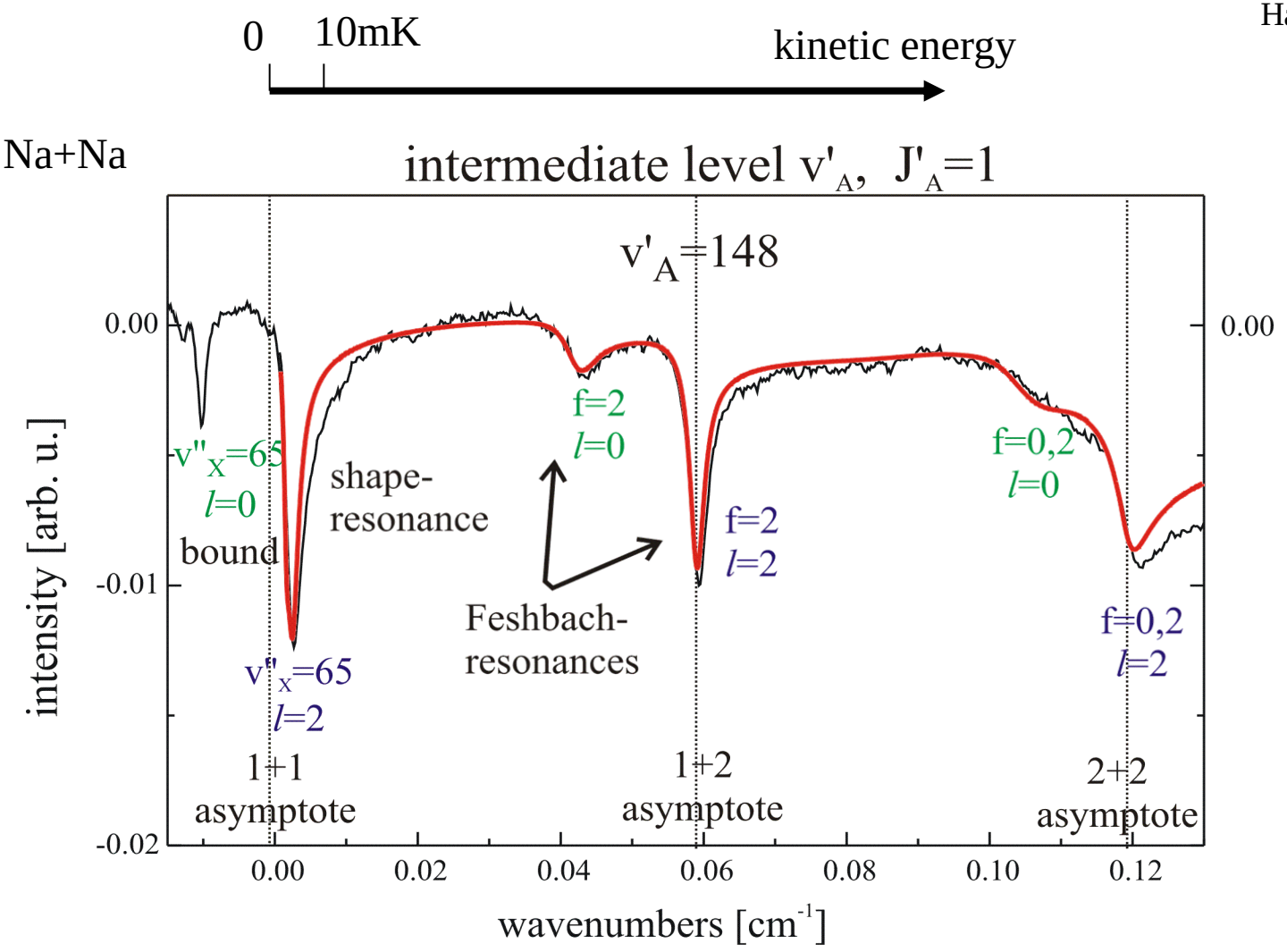

Comparison with simulation

Conclusions

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- studies of ultracold matter demand for new spectroscopy
- complementary experiments in traps and with hot ensembles possible
- evaluation of complete data from different experiments performed

- compact form of huge body of data → molecular potentials, Hamiltonian
- How to keep this information for an easy application for a long time?

developing fields

- wide area of preparing quantum systems with molecules
- using the internal motion in a molecule for precise studies of its dynamic → times dependence of atomic masses?
- ….. never complete