STONY BROOK

Spin-orbit mixing in the $A^1\Sigma^+_u$ and $b^3\Pi_{0u}$ states of Rubidium dimer

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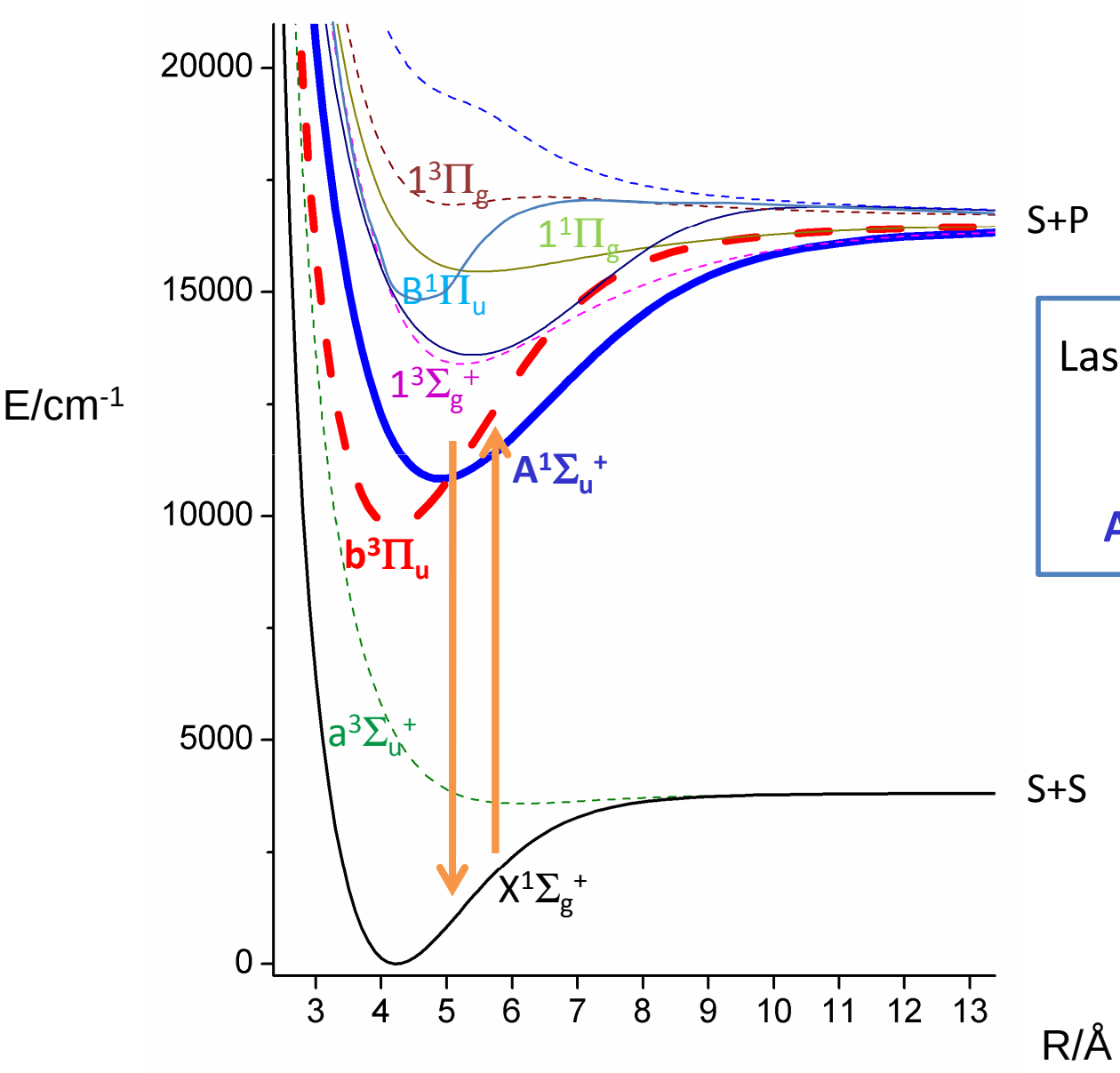
63rd International Symposium on Molecular Spectroscopy, Colombus, June 18, 2008

Investigation of the $A^1\Sigma^+$ and $b^3\Pi$ of Rb_2



Laser Induced Fluorescence

to the ground state

$A^1\Sigma_u^+ \sim b^3\Pi_u \rightarrow X^1\Sigma_g^+$

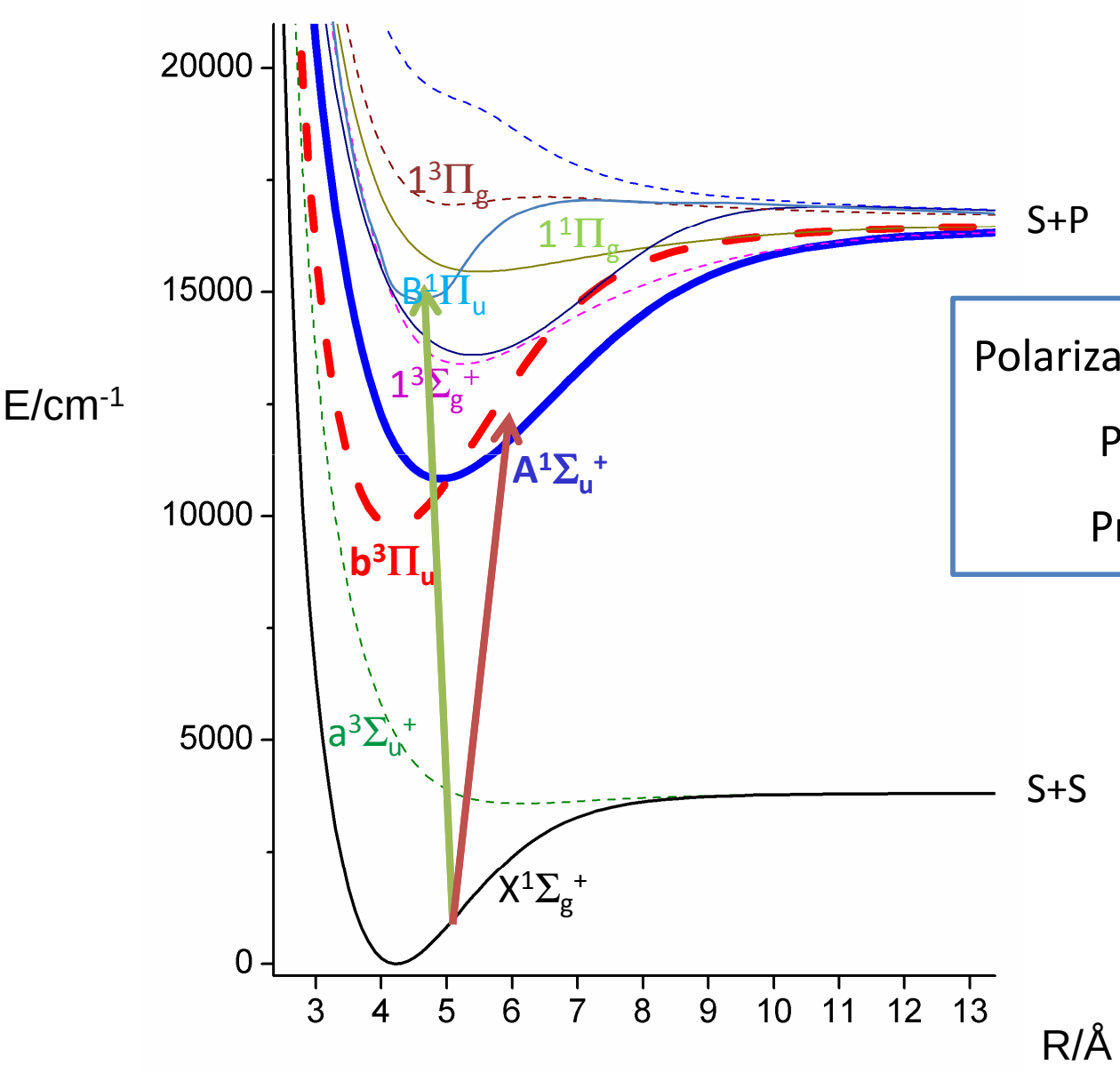
LIF Data from :

Orsay

and recently

Lyon (2008)

Investigation of the $A^1\Sigma^+$ and $b^3\Pi$ of Rb_2



Polarization labeling Spectroscopy

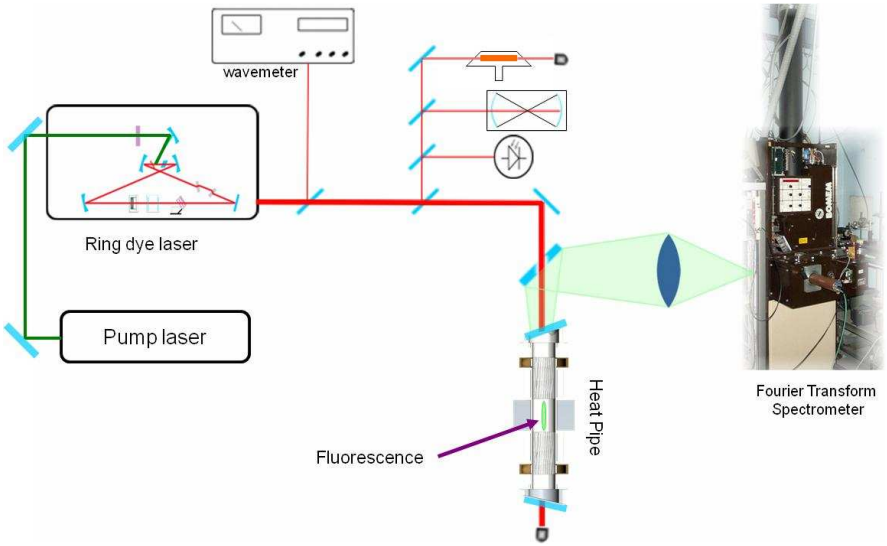
Pump: $X^1\Sigma_g^+ \rightarrow b^3\Pi_u$

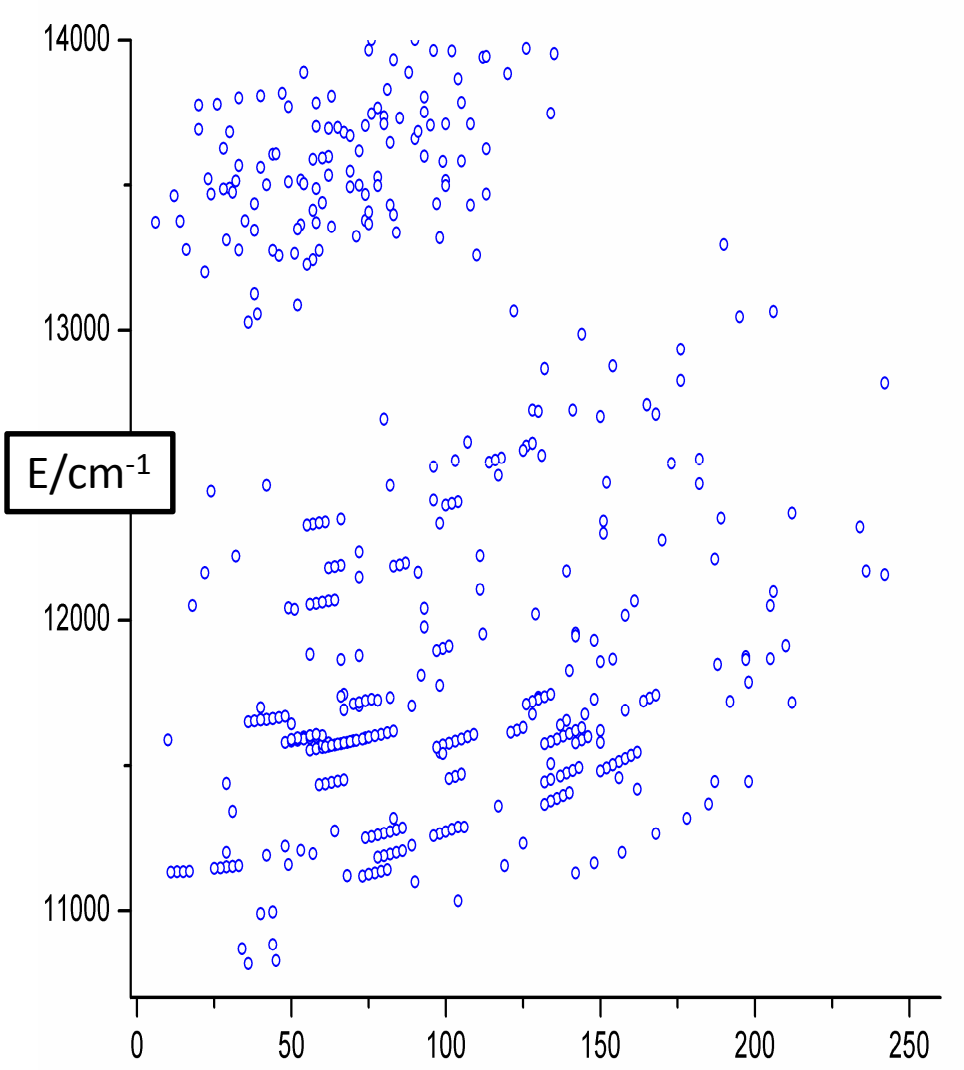
Probe: $X^1\Sigma_g^+ \rightarrow A^1\Sigma_u^+$

Data from:
Temple (2007)

$A^1\Sigma^+ \sim b^3\Pi_{0u}$, Rb_2 data

LIF+FTS: Orsay





$A^1\Sigma^+ \sim b^3\Pi_{0u}$, Rb_2 data

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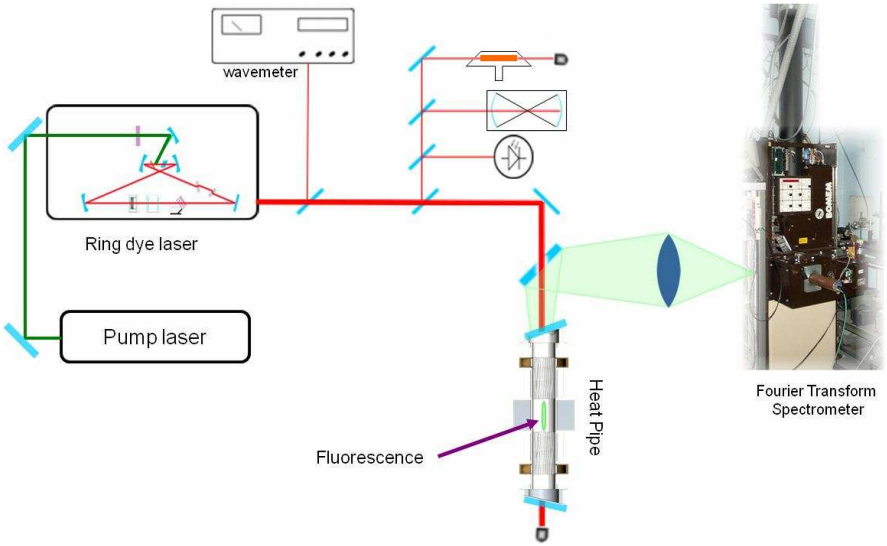
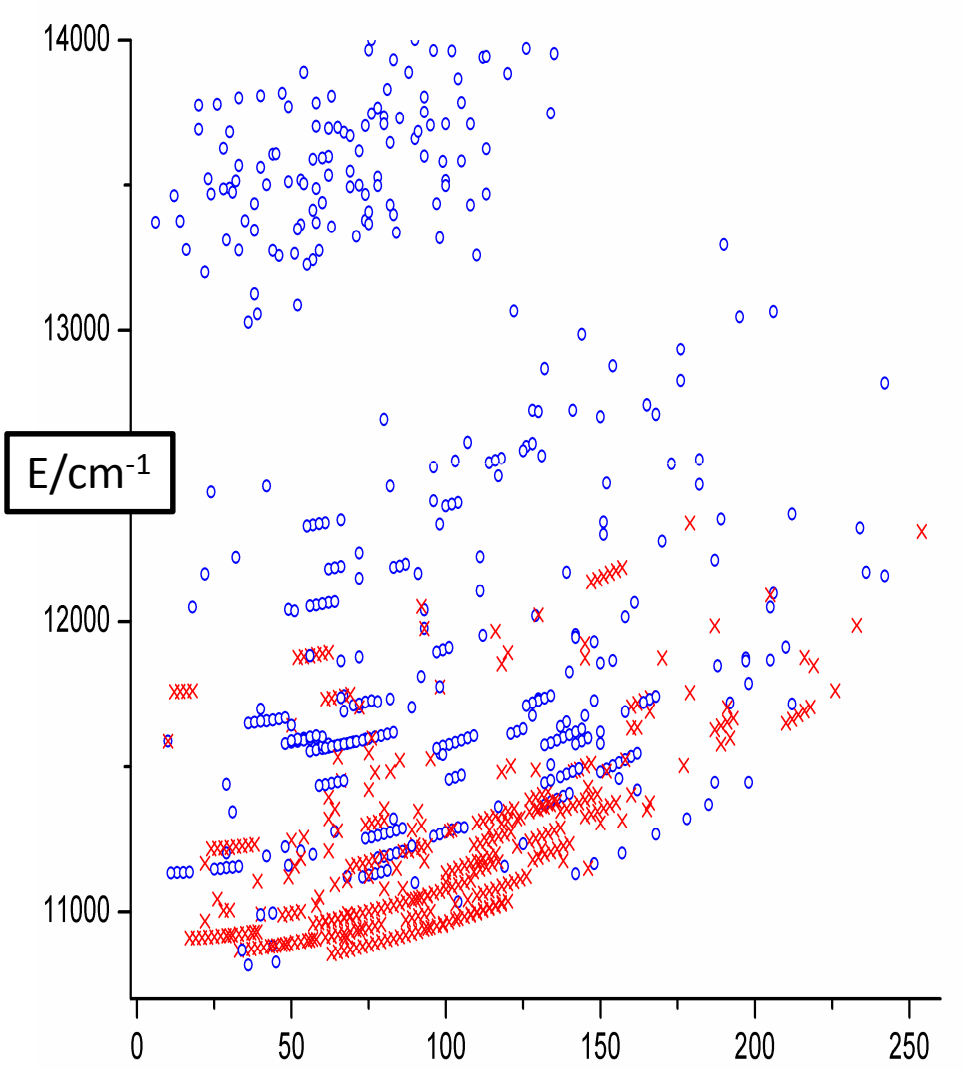
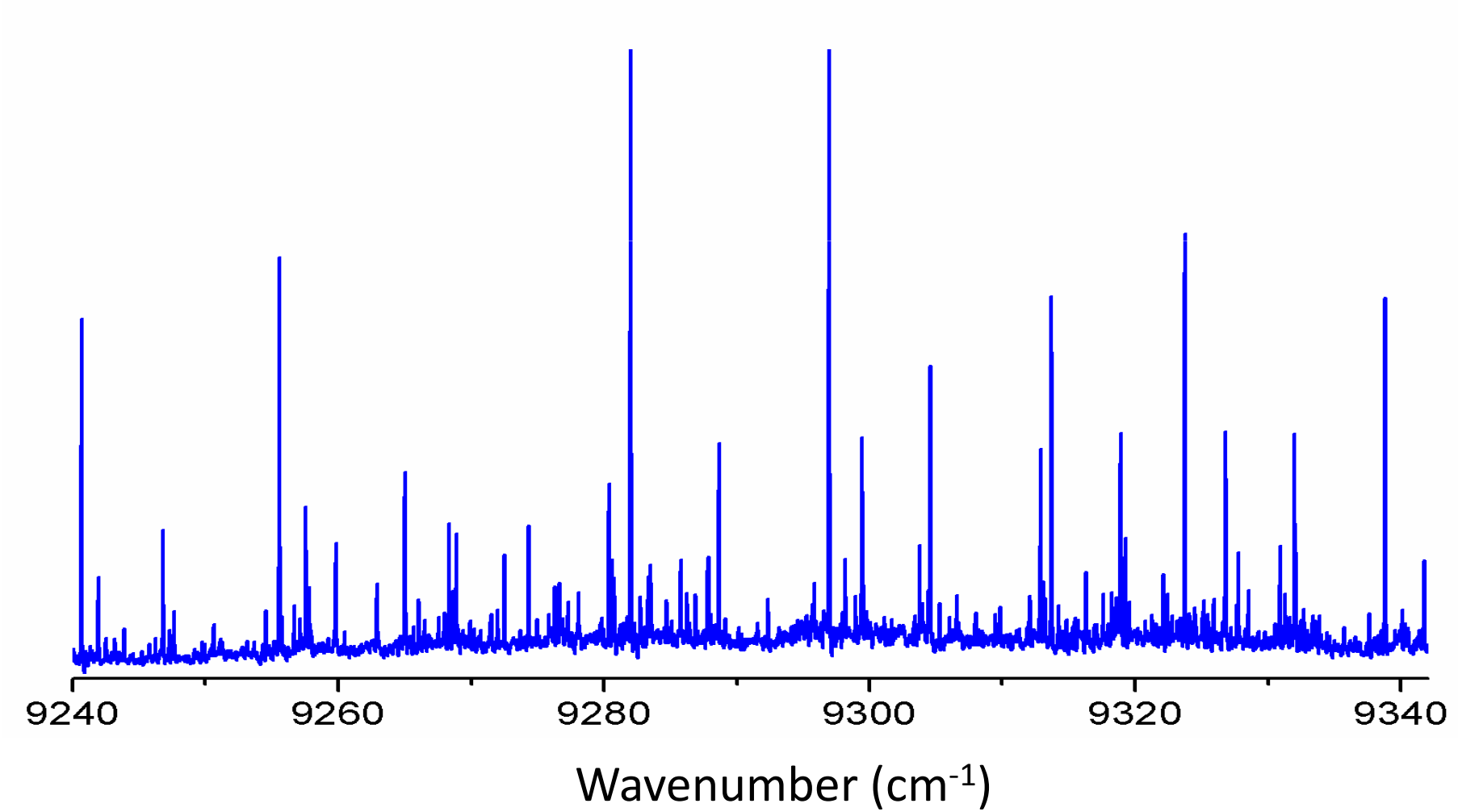




LIF dispersed by Fourier transform spectrometer

Spectrum : A → X fluorescence
excitation laser line : 11150.552 cm^{-1}
Resolution: 0.05 cm^{-1}



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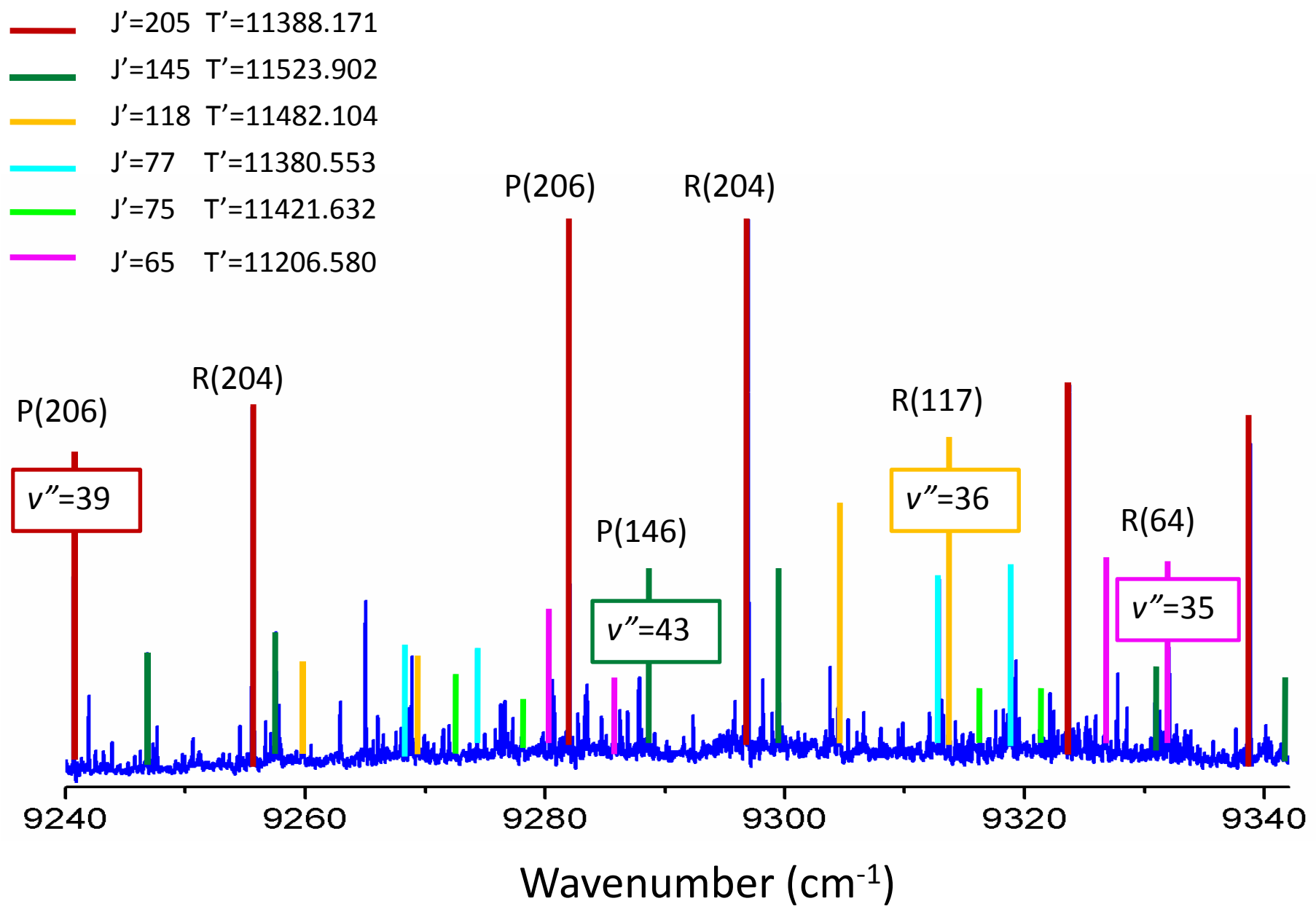

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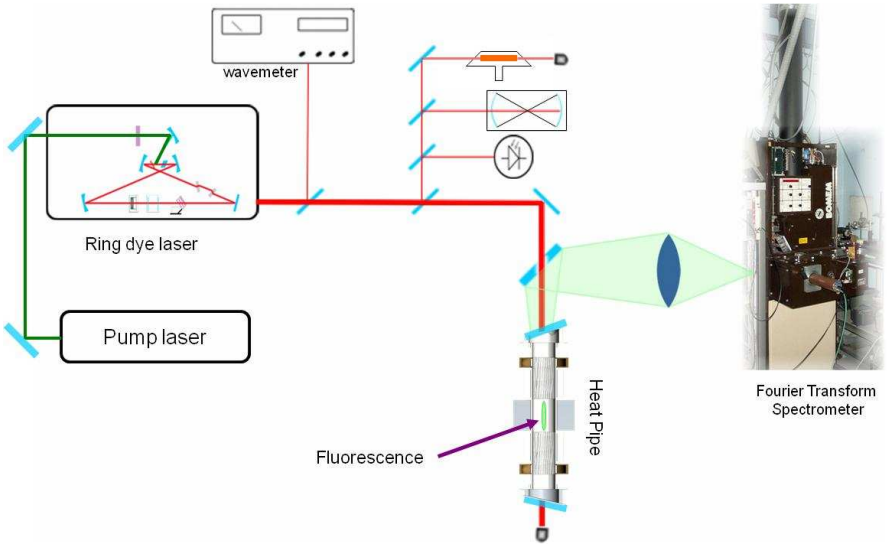

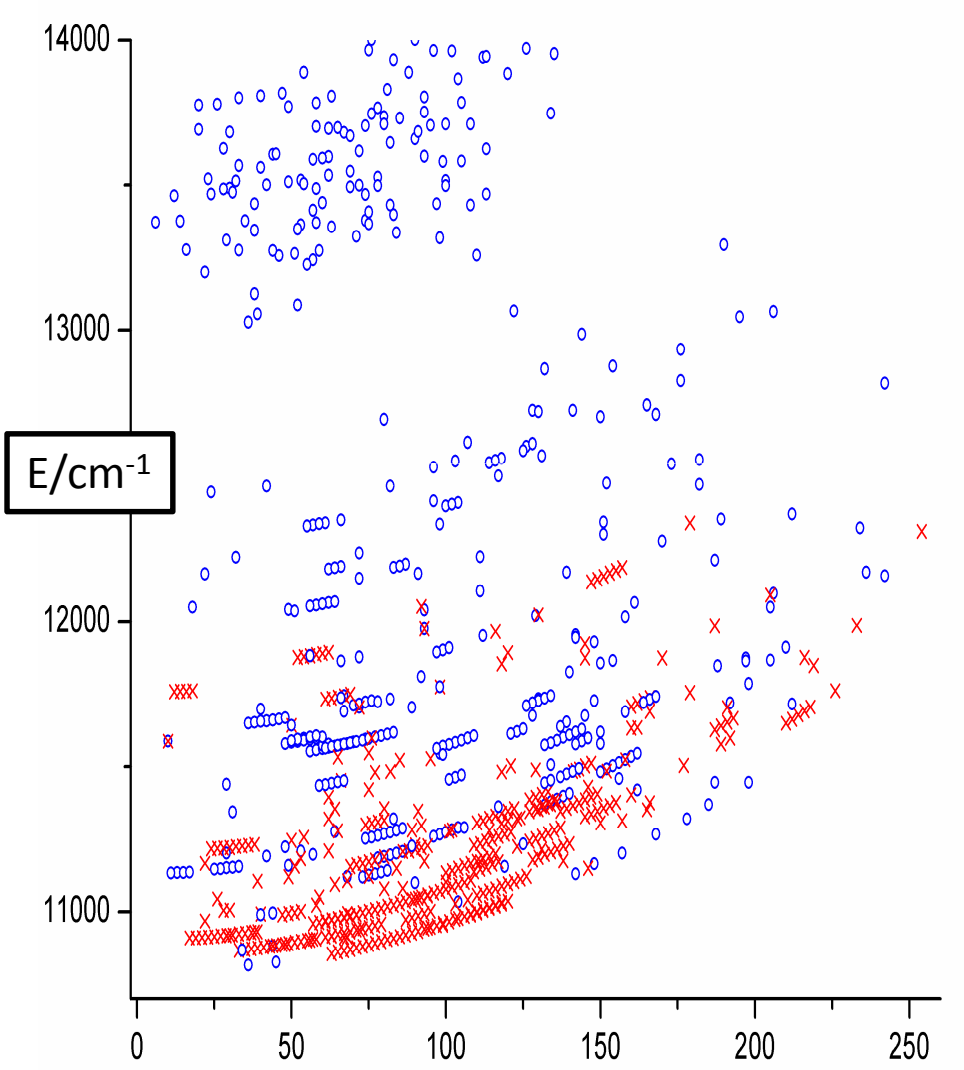

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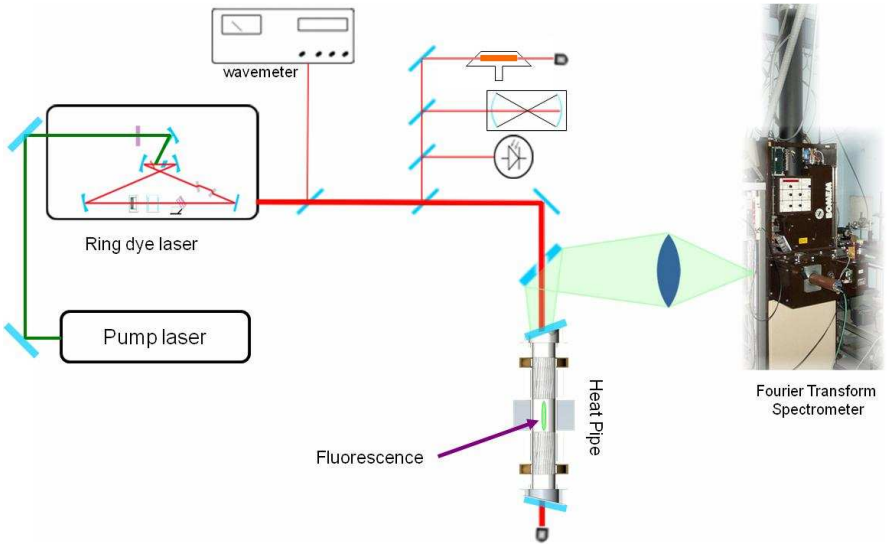
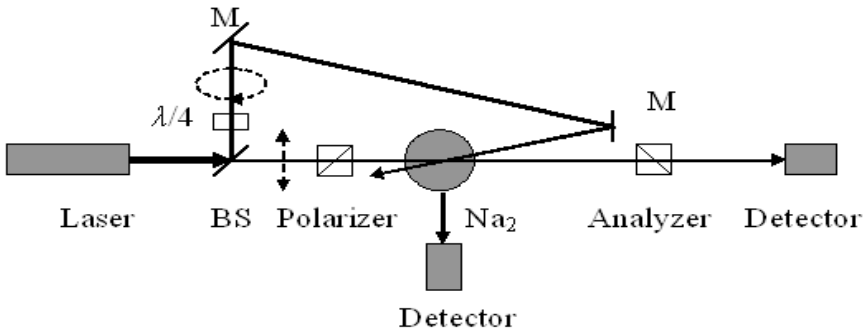
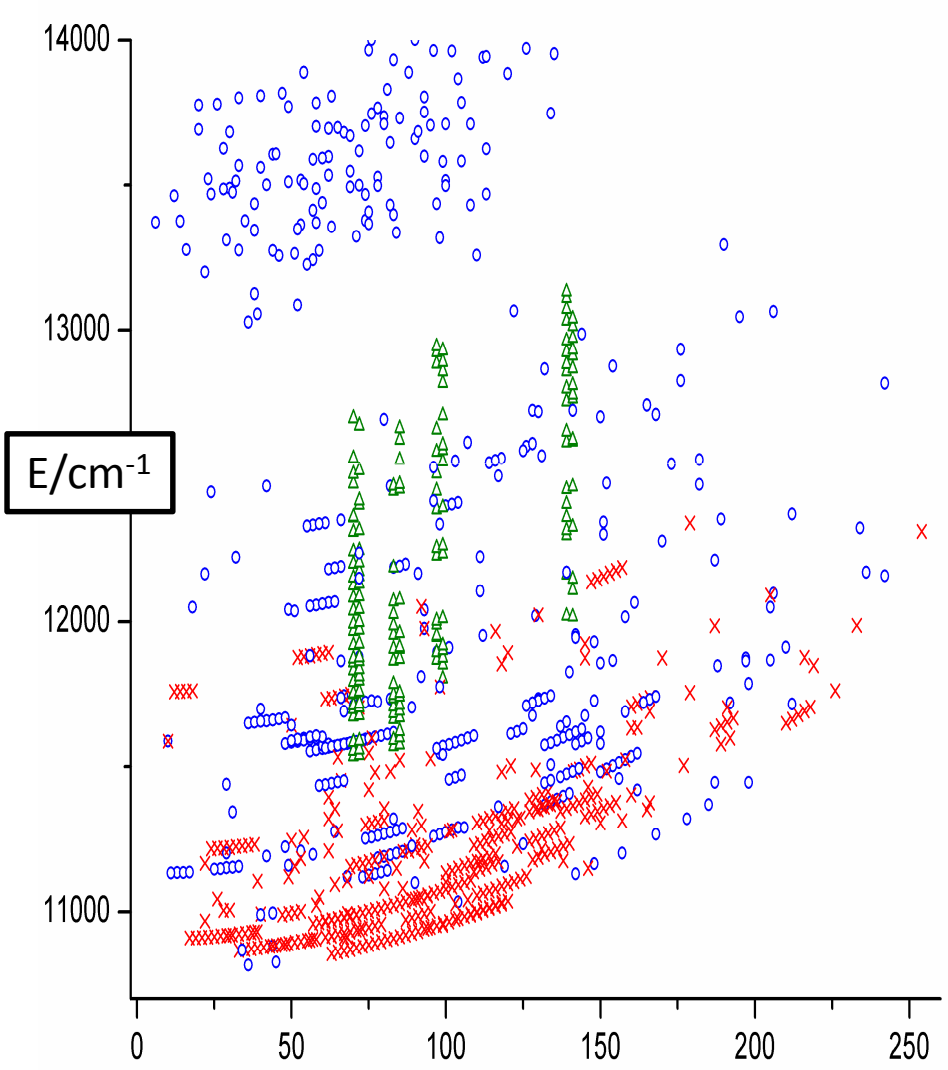


PLS: Temple

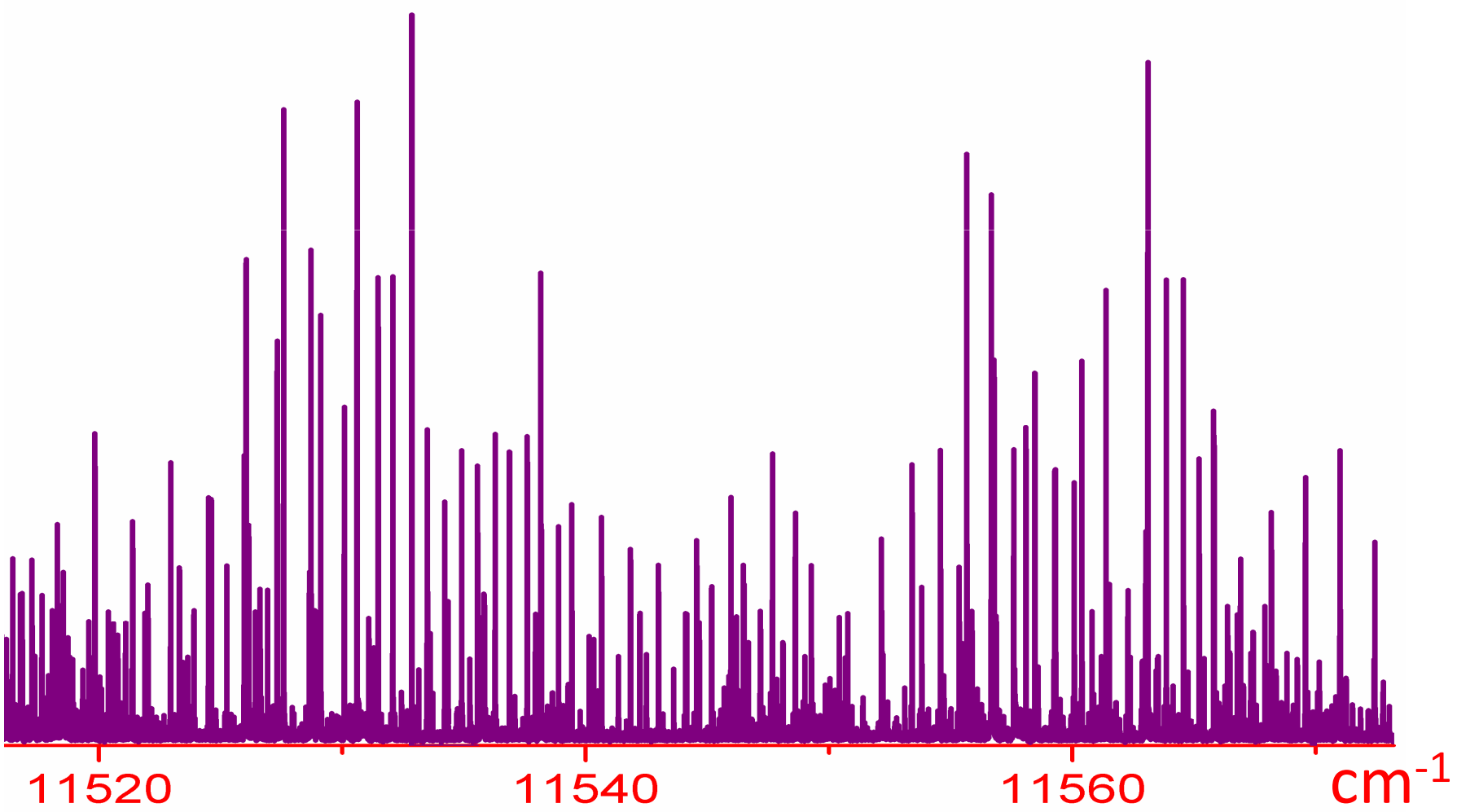




Polarization labeling spectrum

Pump: DCM laser (σ_{laser} = 14736.27 cm^{-1}): $X^1\Sigma_g^+$ (v"=0, J"= 71) → $B^1\Pi_u$ (v'=2, J'=70)

Probe: Ti:Sa laser: $X^1\Sigma_g^+$ → $A^1\Sigma_u^+$



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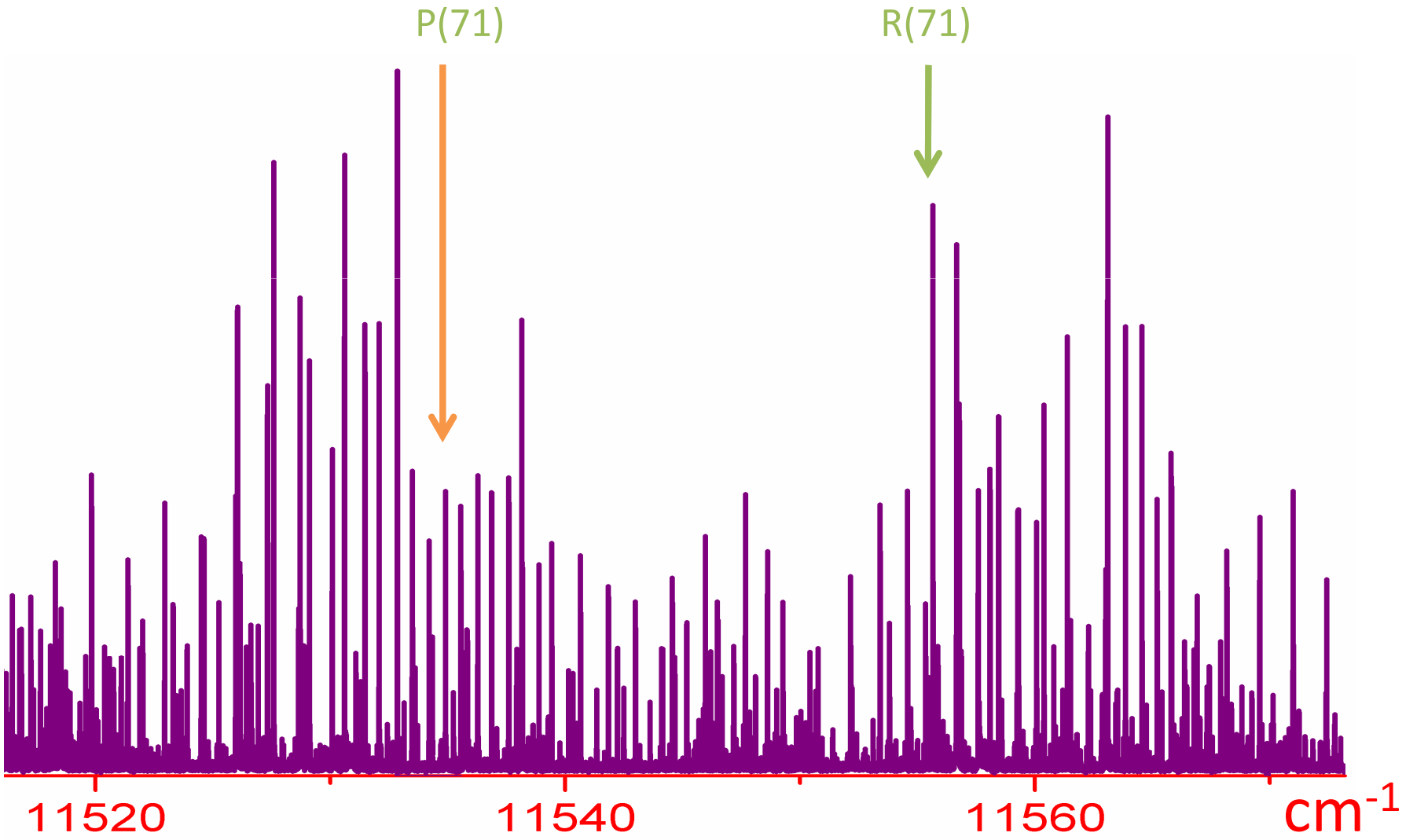

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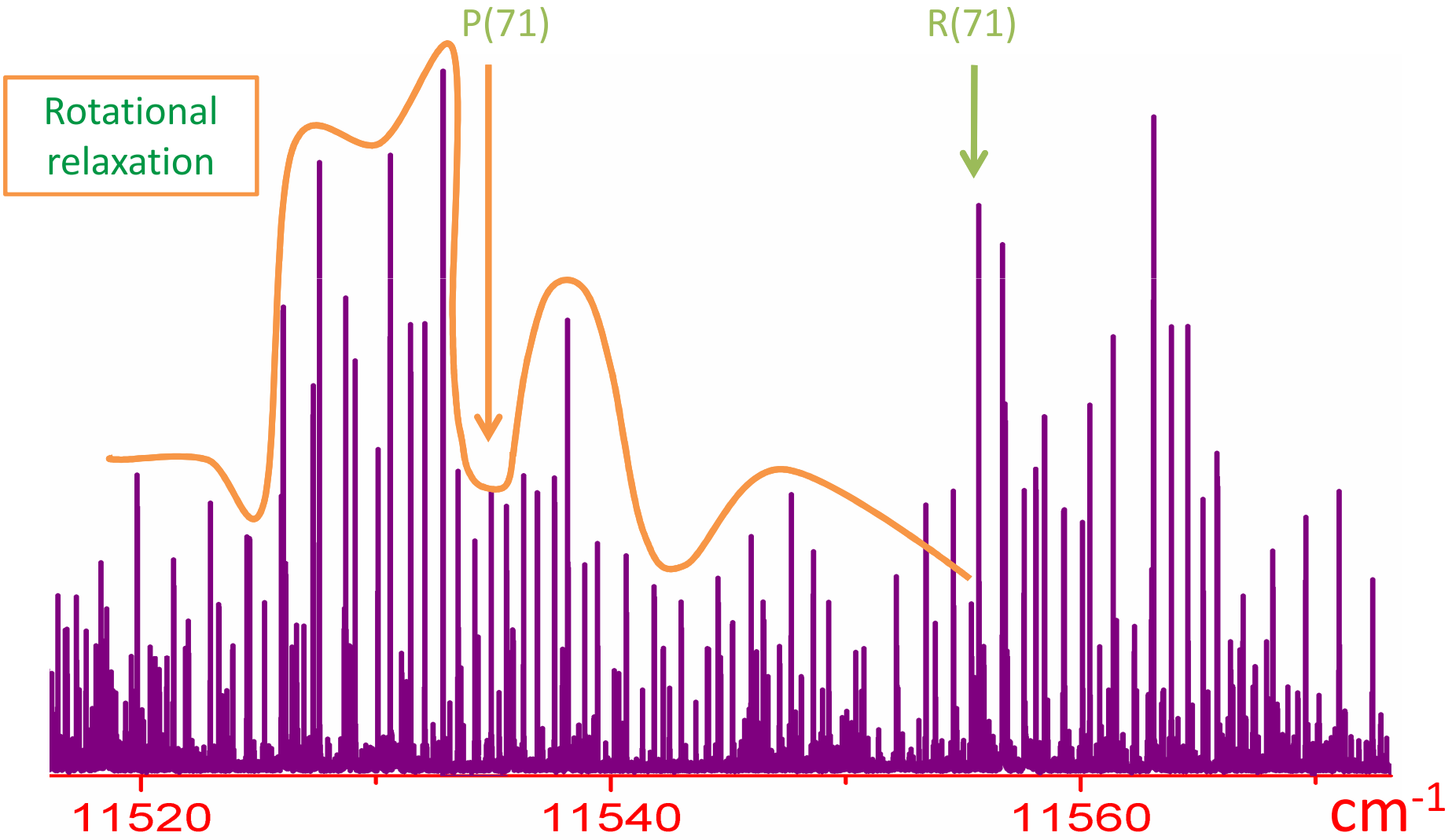

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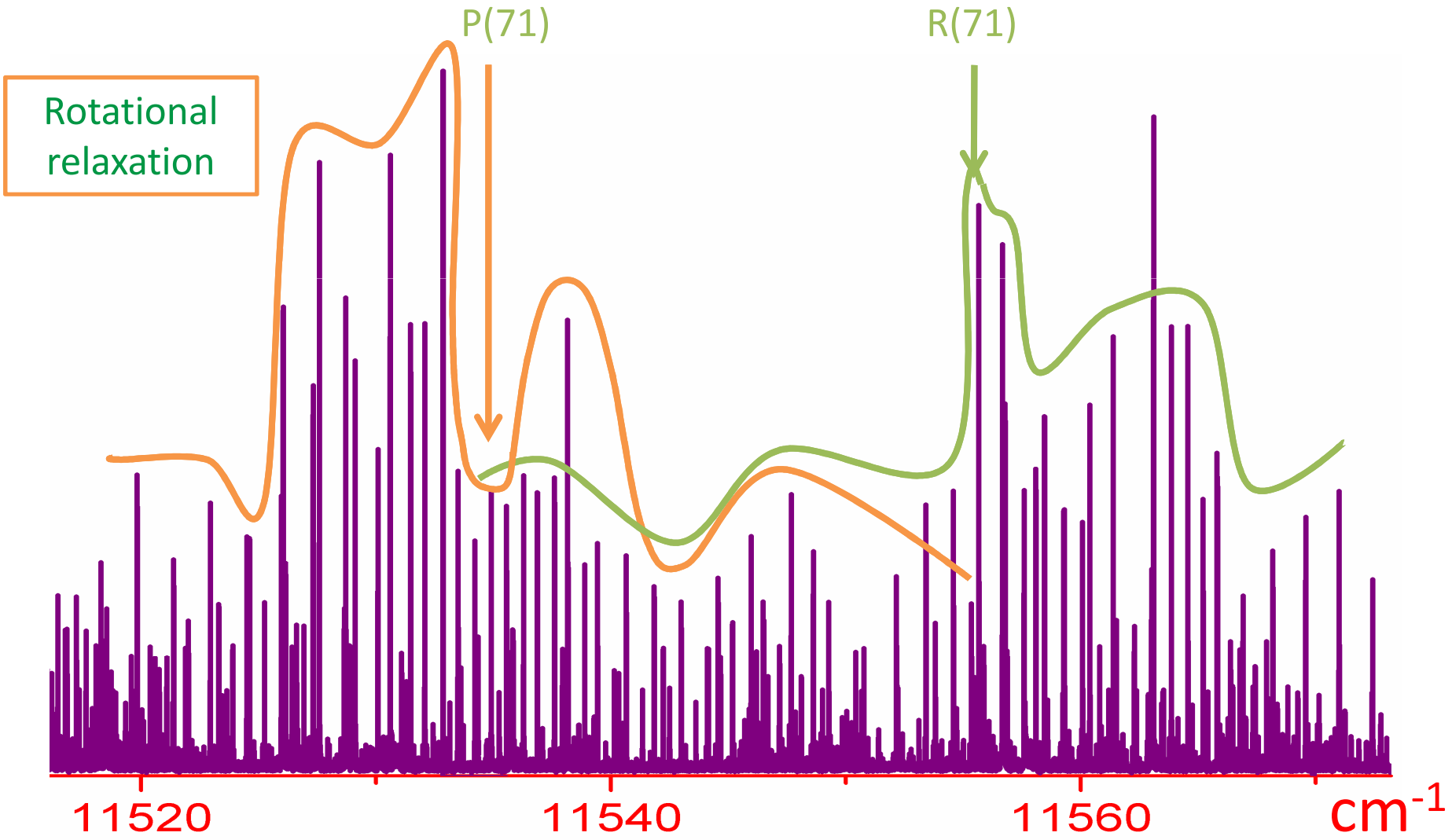
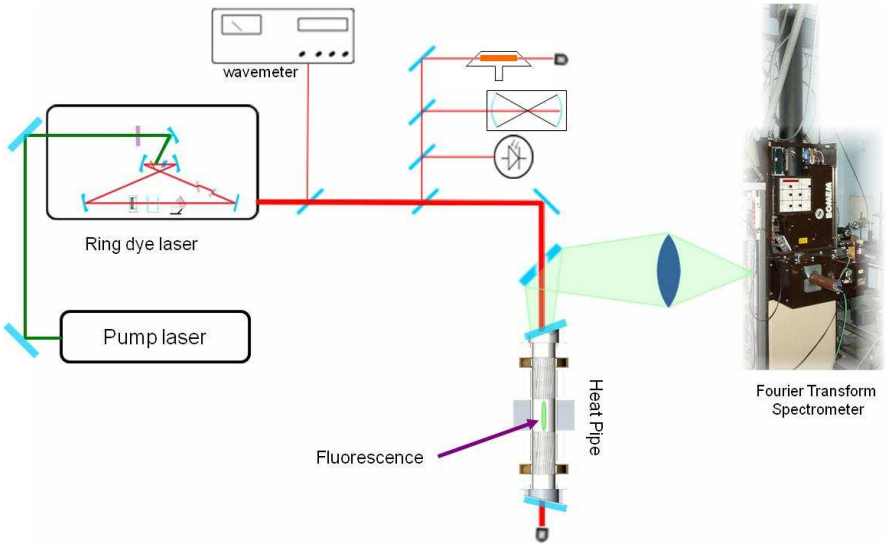
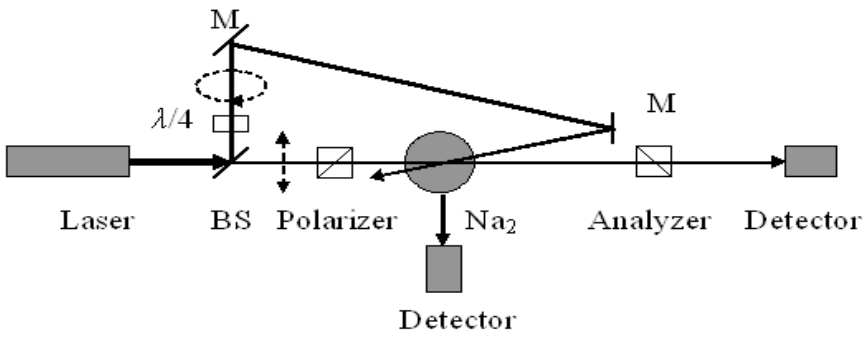


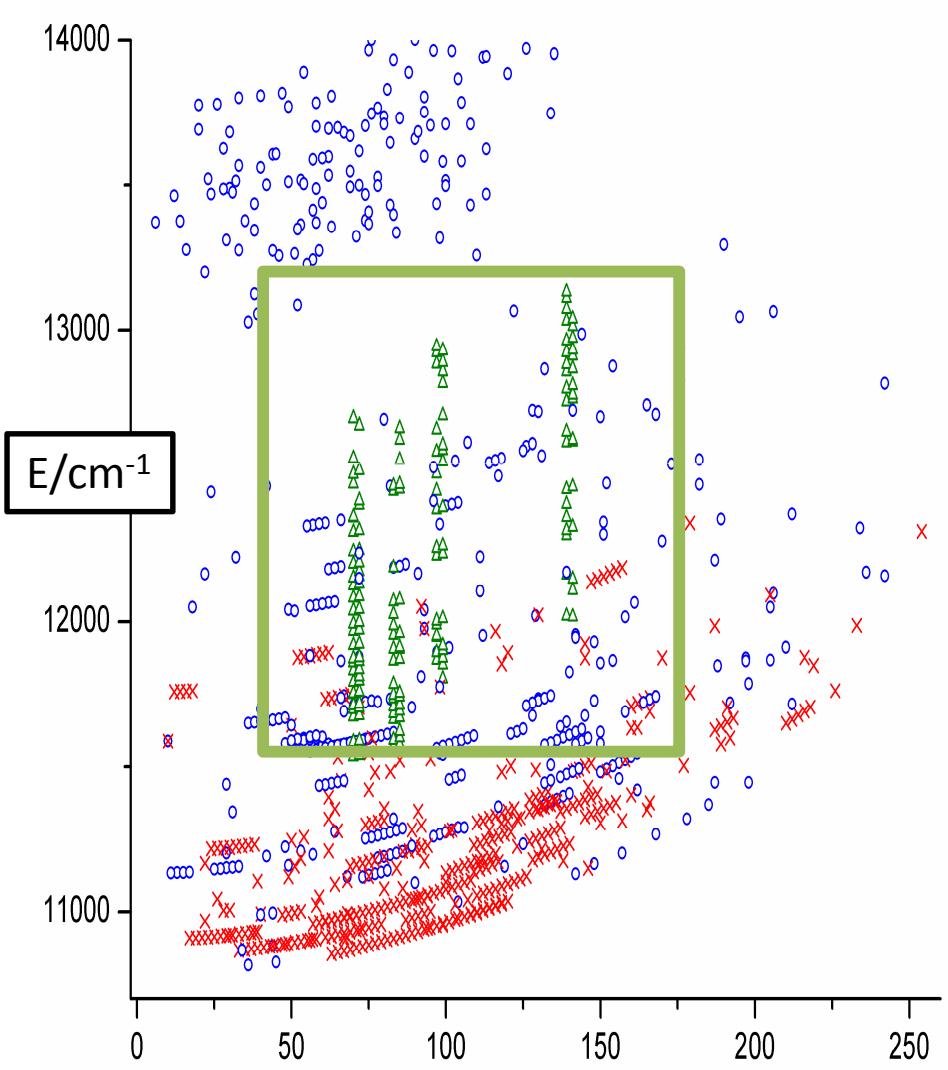
$A^1\Sigma^+ \sim b^3\Pi_{0u}$, Rb_2 data

LIF+FTS: Orsay+Lyon



PLS: Temple





Coupled channel Analysis

Hamiltonian matrix:

$$\begin{array}{c} \\ A^1\Sigma_u^+ \\ b^1\Pi_{0u} \end{array} \begin{array}{c} \begin{array}{cc} A^1\Sigma_u^+ & b^1\Pi_{0u} \end{array} \\ \begin{pmatrix} V\left({}^1\Sigma_u^+\right)+(x+2)B & -\Delta_{od} \\ -\Delta_{od} & V\left({}^1\Pi_u\right)-\Delta_d+(x+2)B \end{pmatrix} \end{array}$$

Potential (Hannover):

$$V(R)=T_e+\sum_{i=2}^{I} a_i\left(\frac{R-R_e}{R+bR_e}\right)^i$$

Spin-Orbit functions:

$$y_{s.o}=(p_1-p_2)\left[1-e^{p_3(R-p_4)}\right]$$

$$p_1=y_{s.o.}(R_m)$$
$$p_2=y_{s.o.}(\infty)=\sqrt{2}\Delta/3$$
$$p_4=R_m$$

Atomic fine structure interval

Parameters in the MLR potential: Ns, NL, p, Φ and in S.O functions

	$A^1\Sigma_u^+$	$b^3\Pi_{0u}$
T_e	10749.735	9598.643
b	0.6	0.3
R_e	4.8737	4.13131
a_3	0.76097D+05	0 .65868D+05
a_4	-0.86239D+05	-0 .33769D+06
a_5	-0.90361D+05	0 .28460D+07
a_6	0.23512D+06	-0.71174D+05
a_7	-0.13456D+07	-0.11185D+09
a_8	0.94888D+07	0.54340D+09
a_9	-0.23772D+07	-0.83496D+09
a_{10}	-0.18889D+09	-0.19643D+09
a_{11}	0.44567D+09	0.62084D+09
a_{12}	-0.64269D+08	0.12395D+10

$$V(R) = T_e + \sum_{i=2}^{I} a_i \left(\frac{R - R_e}{R + bR_e} \right)^i$$

Spin-orbit Function

$$y_{s.o} = p_1 + (p_2 - p_1)\left[1 - e^{p_3(p_4 - R)}\right]$$

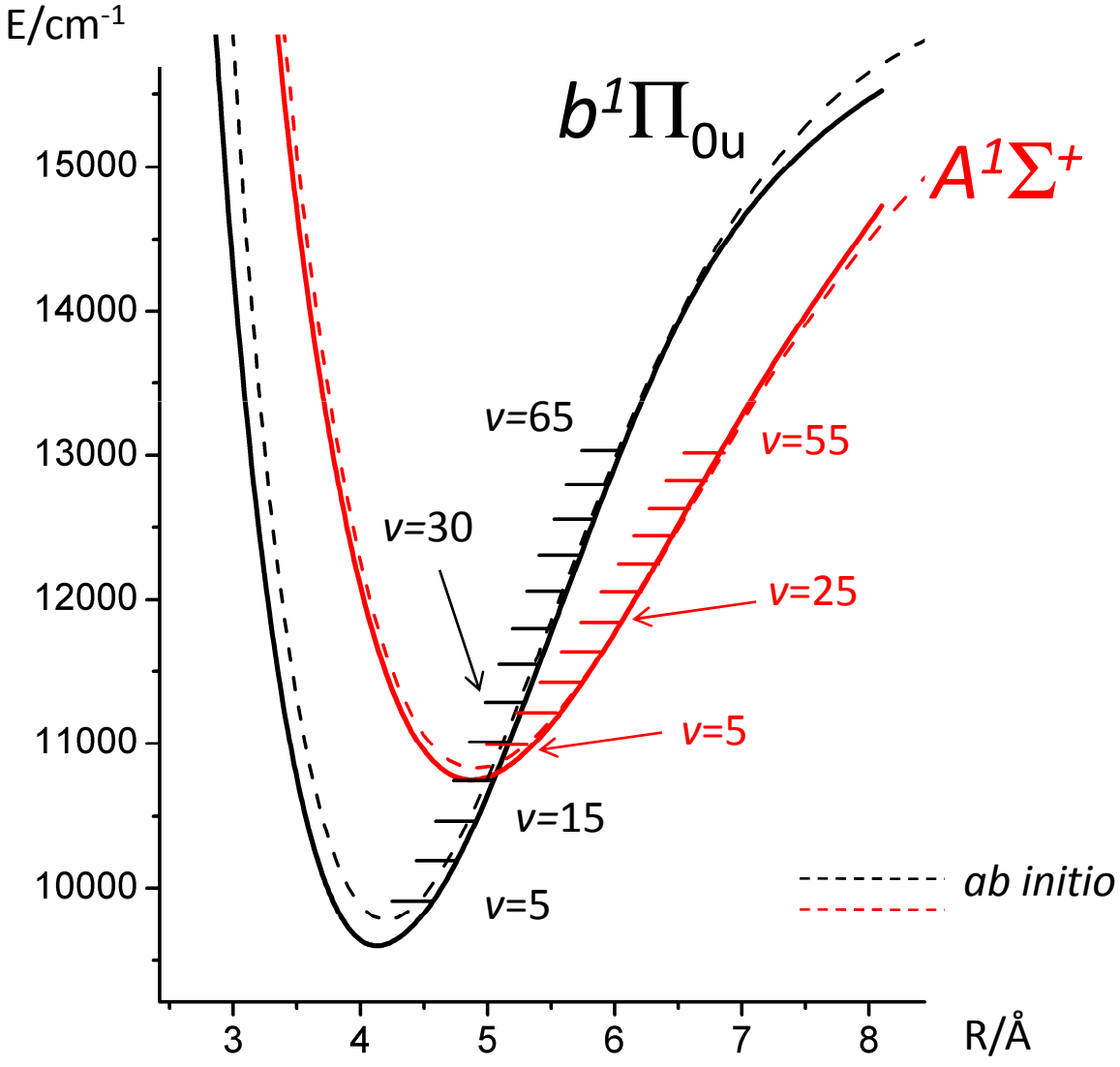
$$p_1 = y_{s.o.}(R_m) = 74.9(4)$$

$$p_2 = y_{s.o.}(\infty) = 112.005$$

$$p_3 = 0.400(5)$$

$$p_4 = R_m = 5.50(1)$$

Fitted potentials



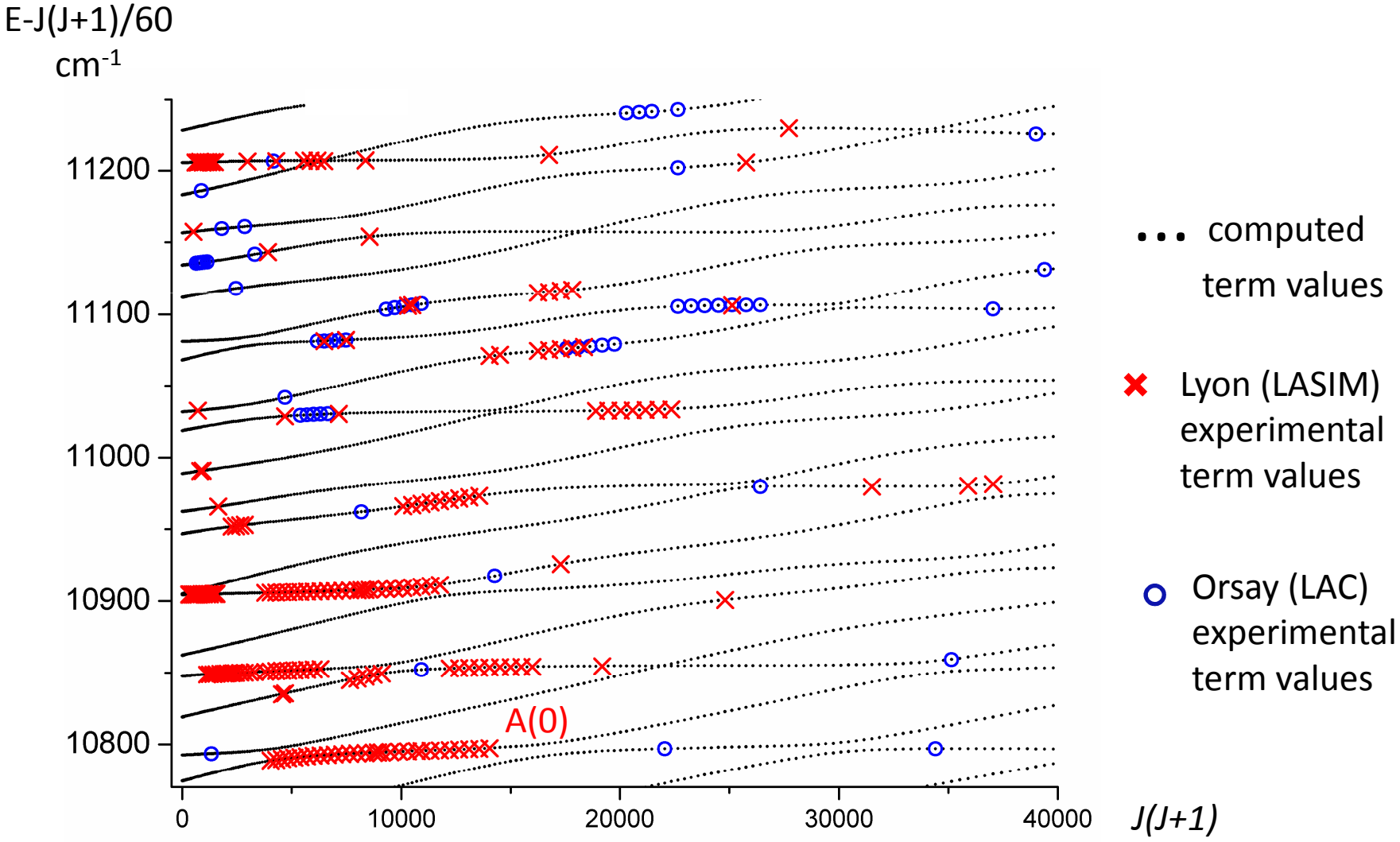
Confirmed absolute vibrational numbering for the $A^1\Sigma^+$ state.

The vib. assignment in the $b^1\Pi_{0u}$ state is convincing but is not definitive.

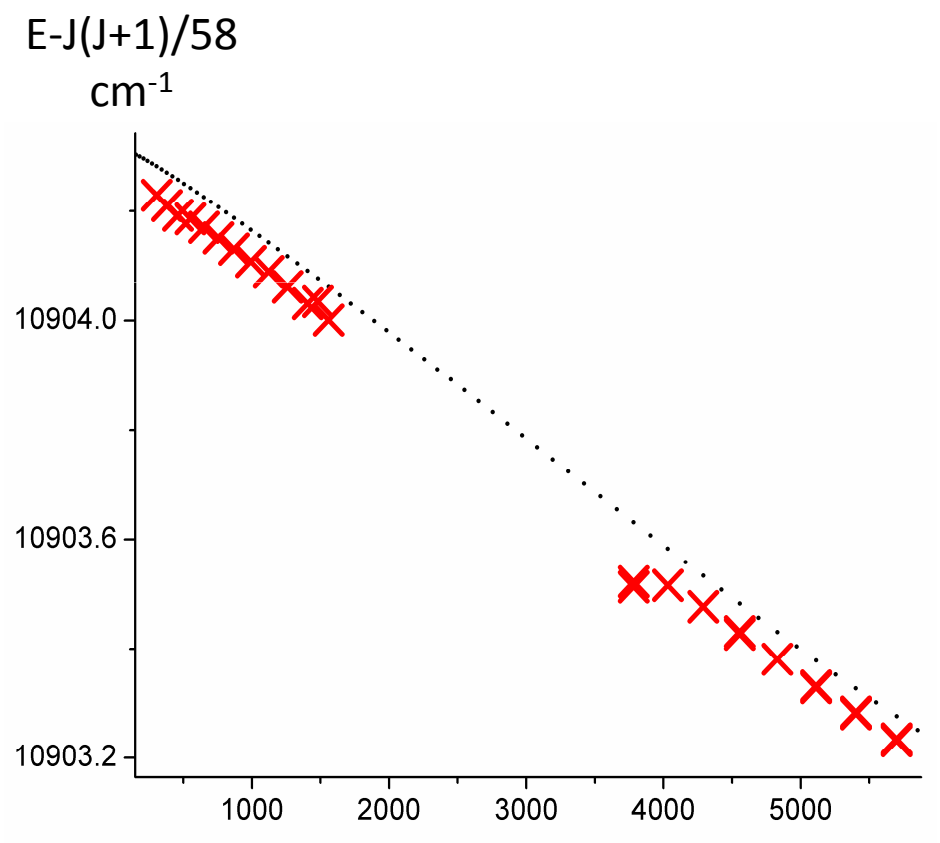
Term Values

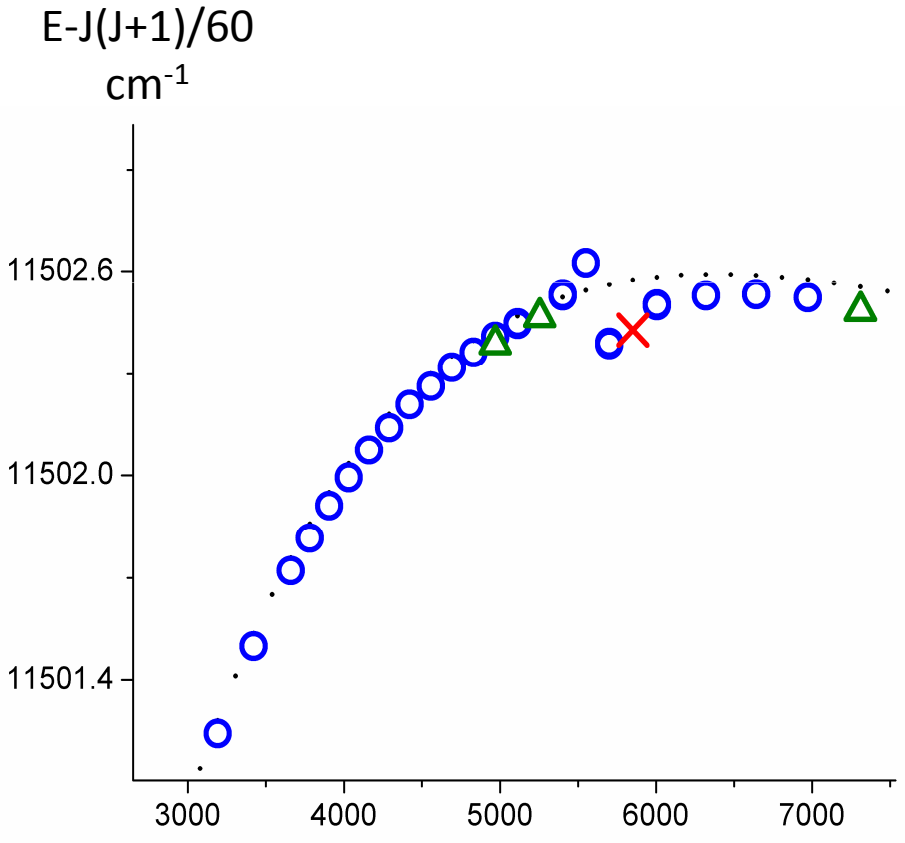
Root mean square deviation = 0.07 cm^{-1},

~ 12 times more than the experimental uncertainty



Avoid crossing?
Due to $b^3\Pi_{0u}$ or $b^3\Pi_{1u}$





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- **A. M. Lyyra, S. Kotochigova, B. Beser, J. Bai, Temple U.**
- **O. Dulieu**

Thank you for your attention