Study of B-like ions X-ray Emission Spectra in an Electron-Cyclotron Resonance Ion Source plasma

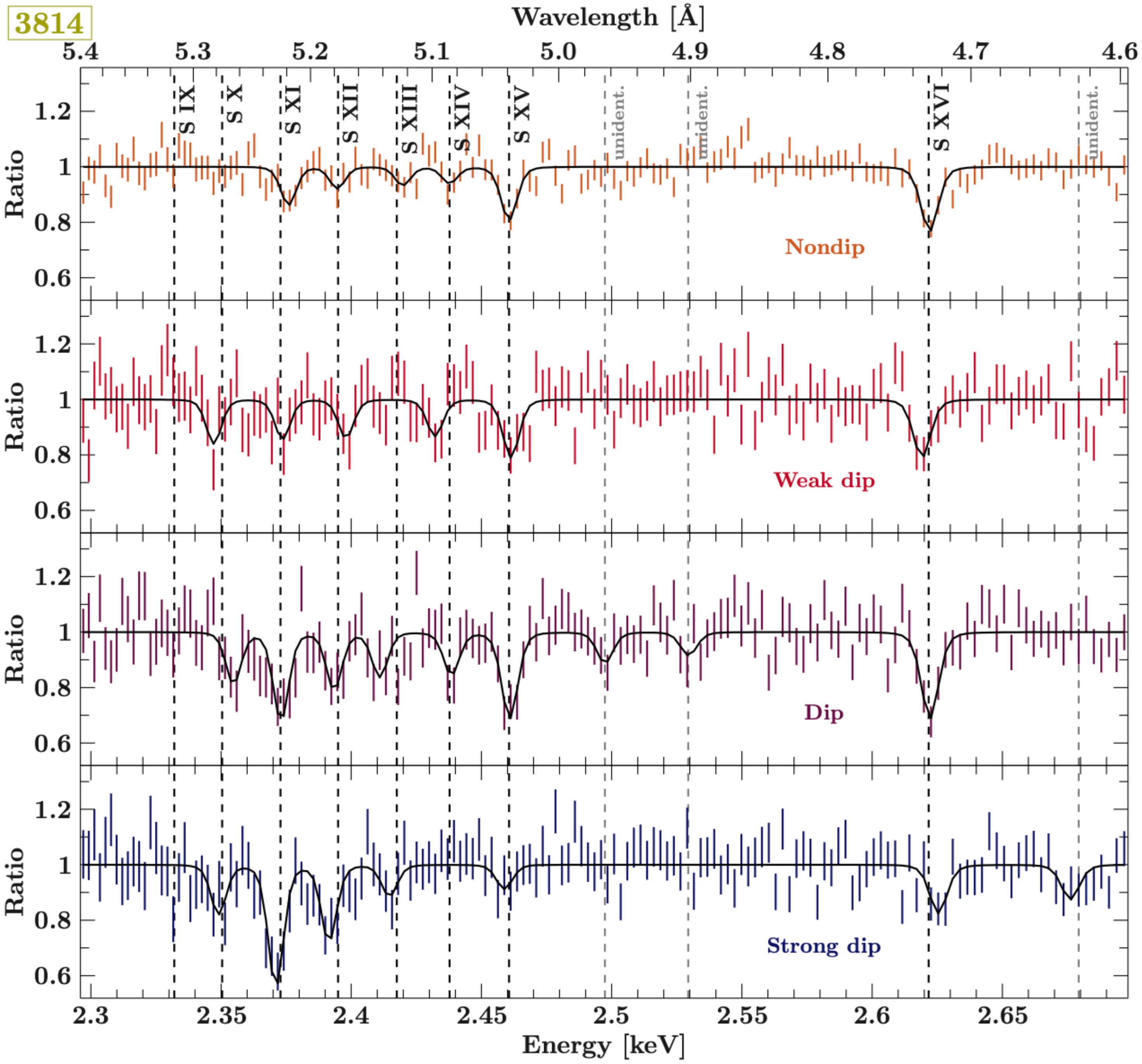
Louis Duval, Jorge Machado, Martino Trassinelli, Nancy Paul, Paul Indelicato

Summary

- Astrophysics and Highly Charged Ions (HCI)
- Boron-like Argon and Sulfur
- Bayesian data analysis
- Preliminary results

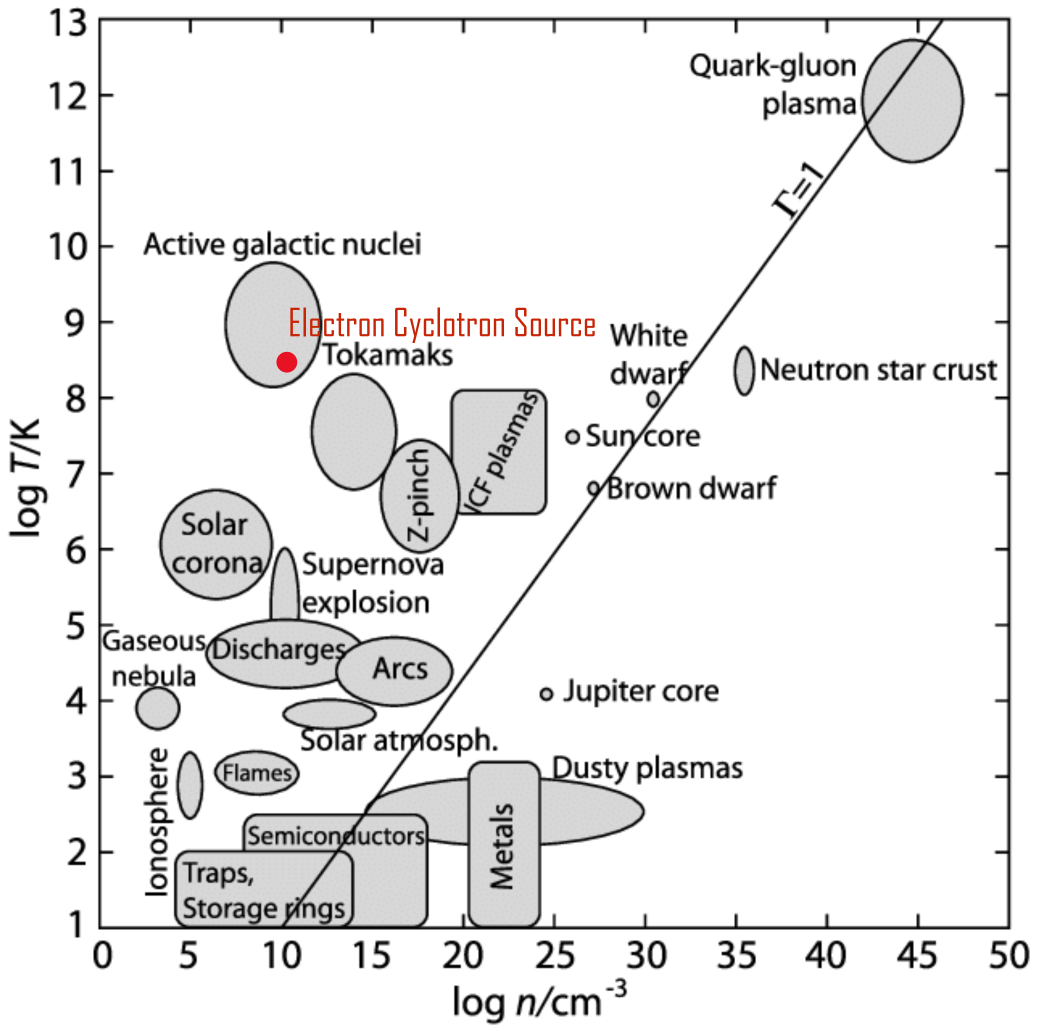
Sources of Highly Charged Ions

- Absorption or emission of sulfur
- black hole binary Cyg X-1/HDE 226868
- Bumps or holes are signatures from inhomogeneities in temperature and densities in the stellar wind powered by the accretion



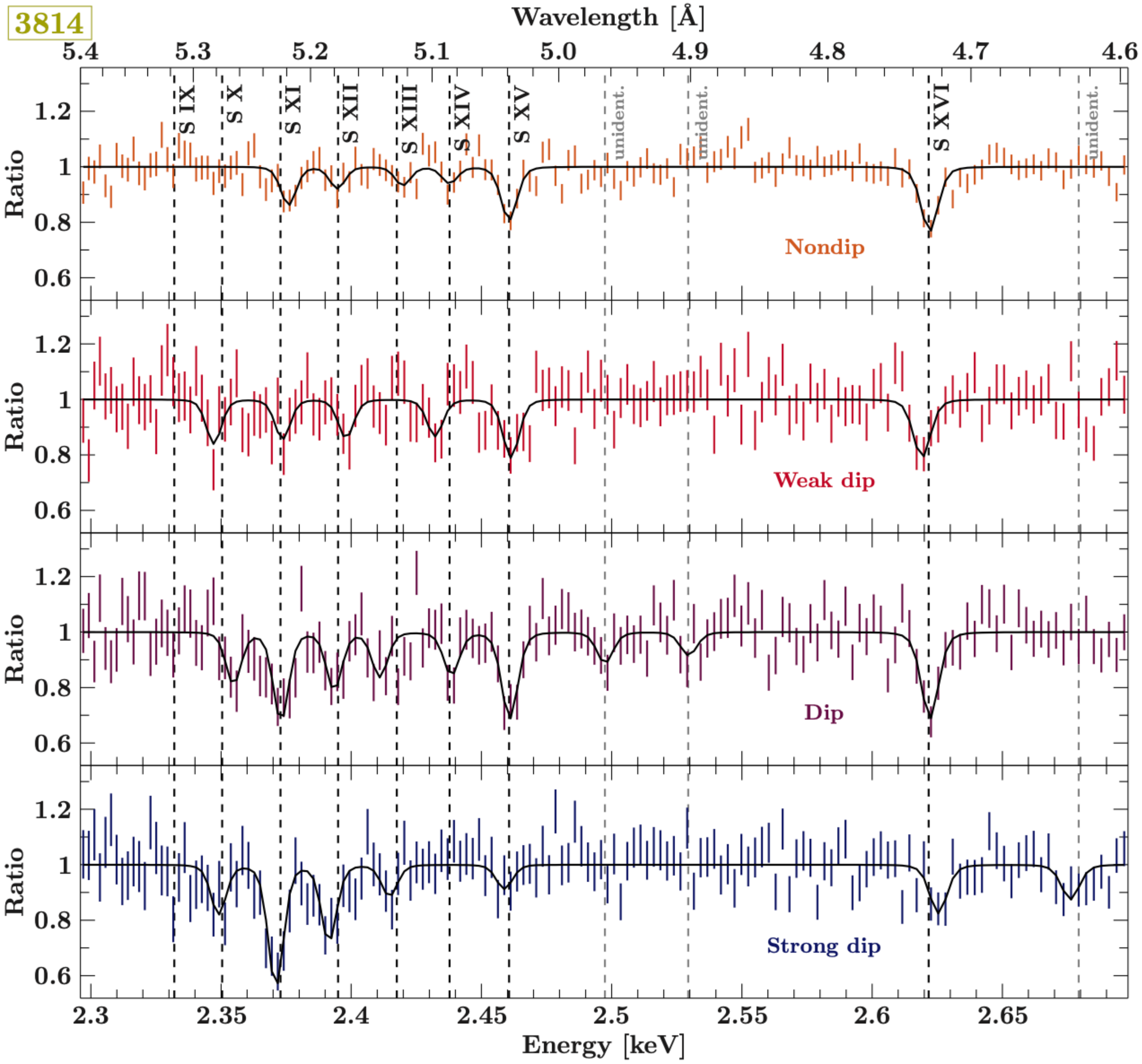
M. Hirsch, N. Hell, V. Grinberg *et al,* A&A 626, A64 (2019)

Sources of Highly Charged Ions



Temperature and electron densities of different plasmas

Donkó, Hartmann and Kalman. (**2007**). Strongly Coupled Plasma Liquids.



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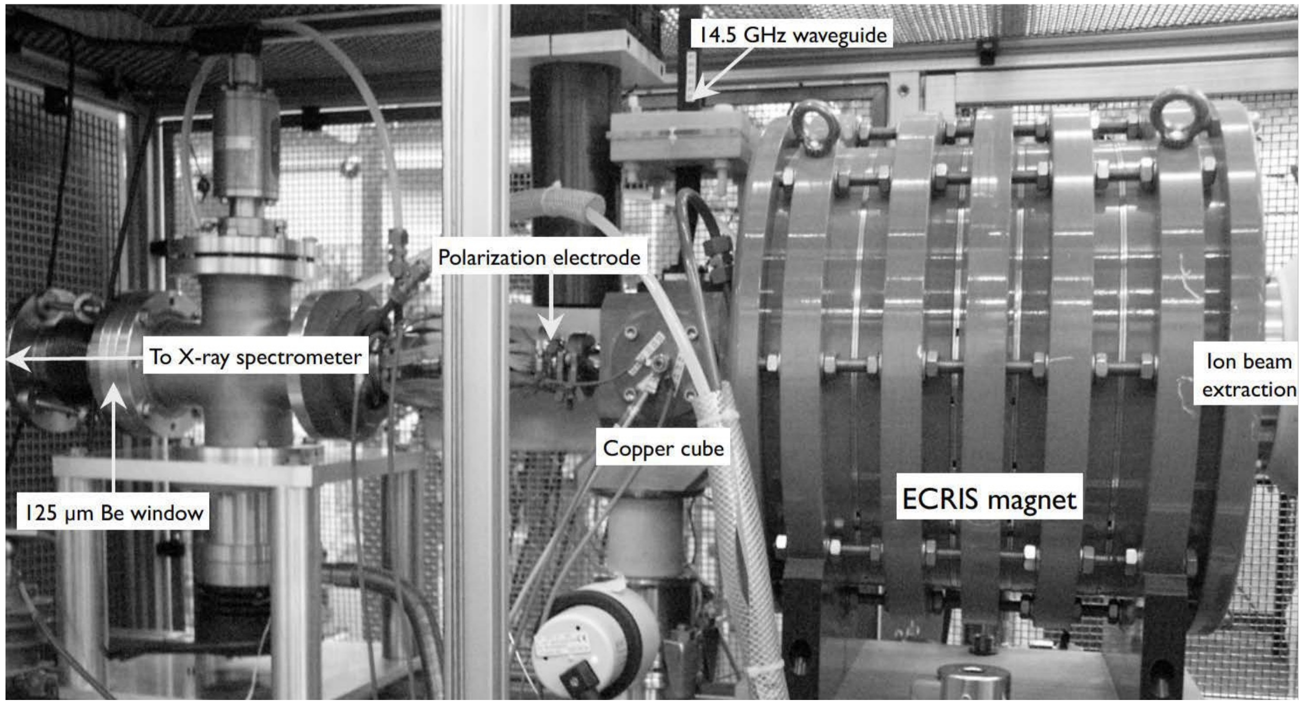
Source d’Ions Multichargés de Paris (SIMPA)



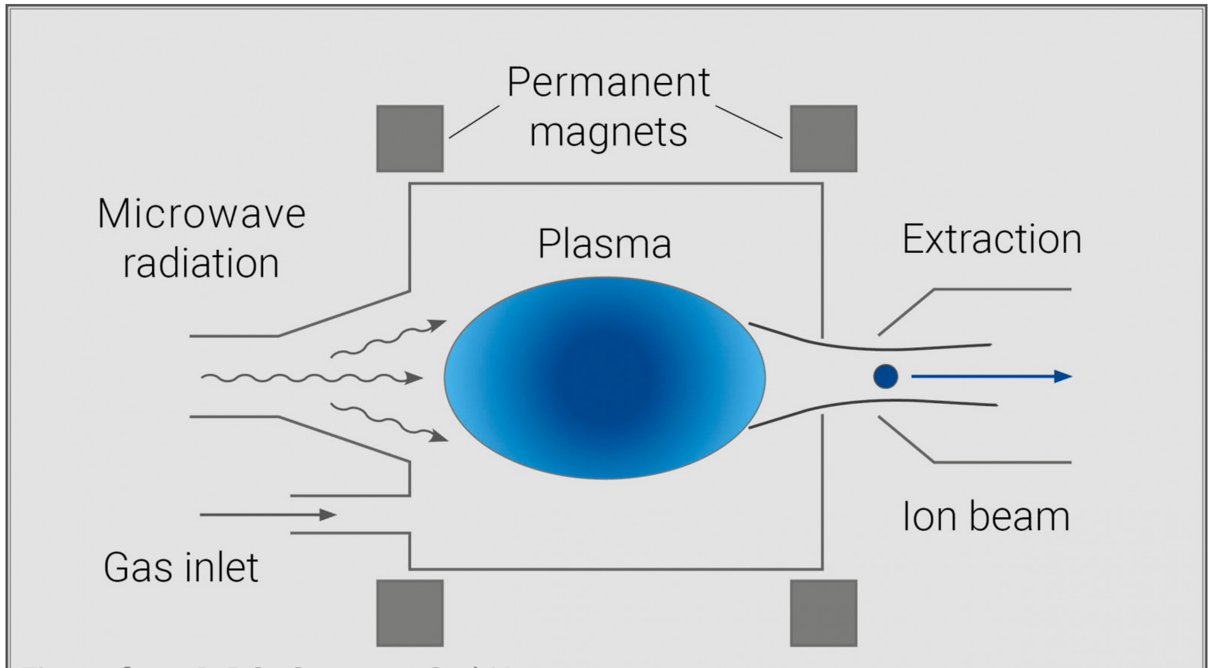
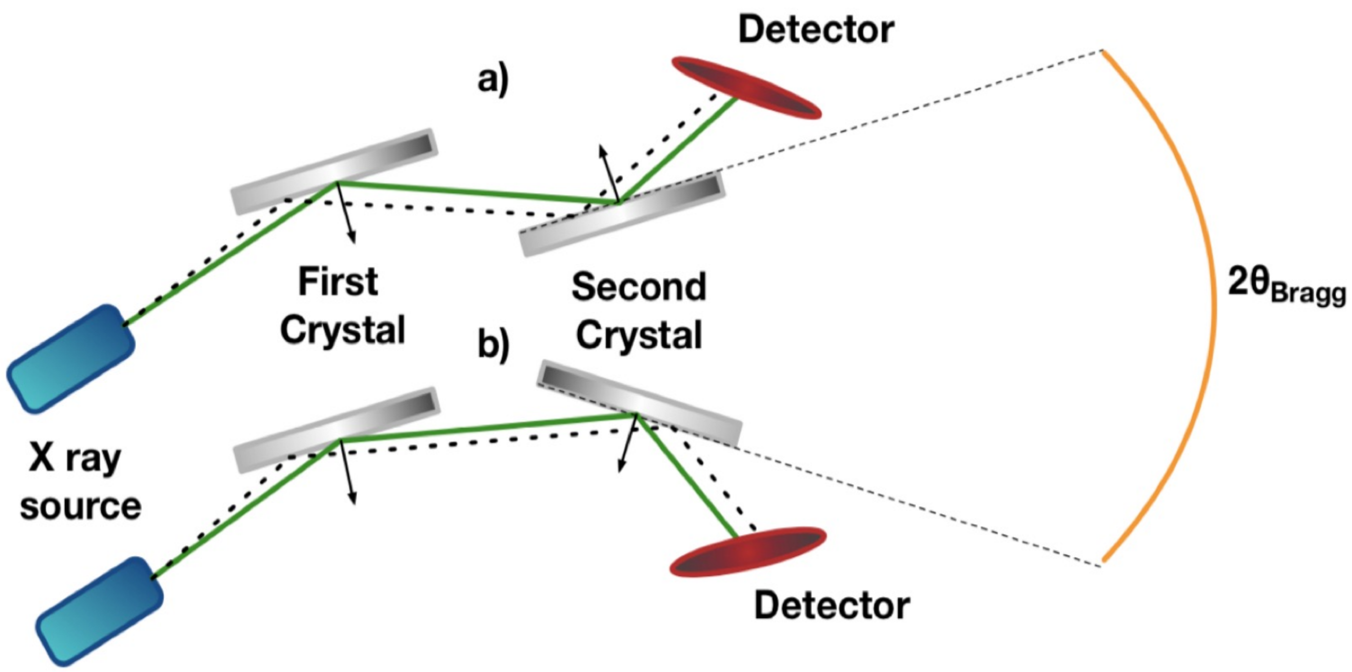


Figure from D.I.S. Germany GmbH

- Production of ions up to H-like Argon
- Direct connection to plasma, 50μm thick Be window
- Microwaves: 14.5 GHz
- Extraction Voltage: up to 25 kV

- In the plasma the ions are trapped in the space charge of the electrons (~10^{11} e-/cm3), ~ few eV trapping depth.
- Electron temperature ~20keV- 10^{8} K
- Intense source, provides access to forbidden transitions, narrow linewidths

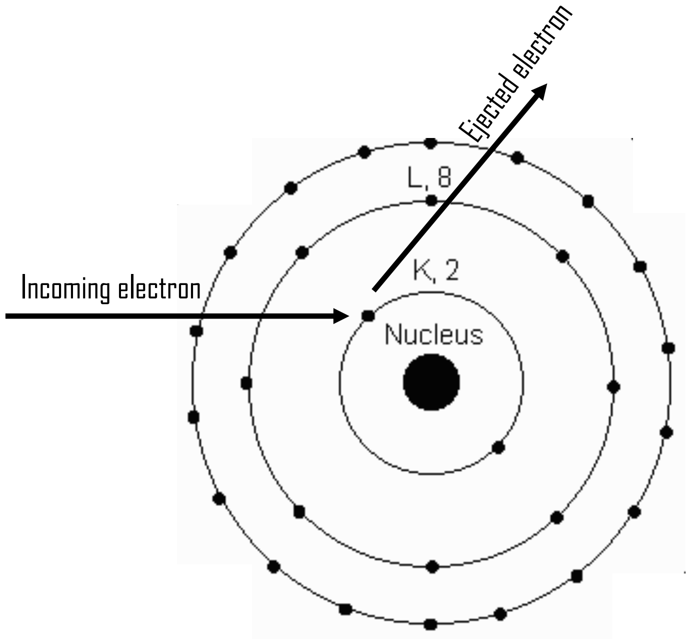
Double Crystal Spectrometer (DCS)



Bragg's law:

$$2d \sin \theta = n\lambda$$

- Double Crystal Spectrometer
- Installed at the **ECR** source **SIMPA**
- **Reference free** measurement
- **Ppm** precision

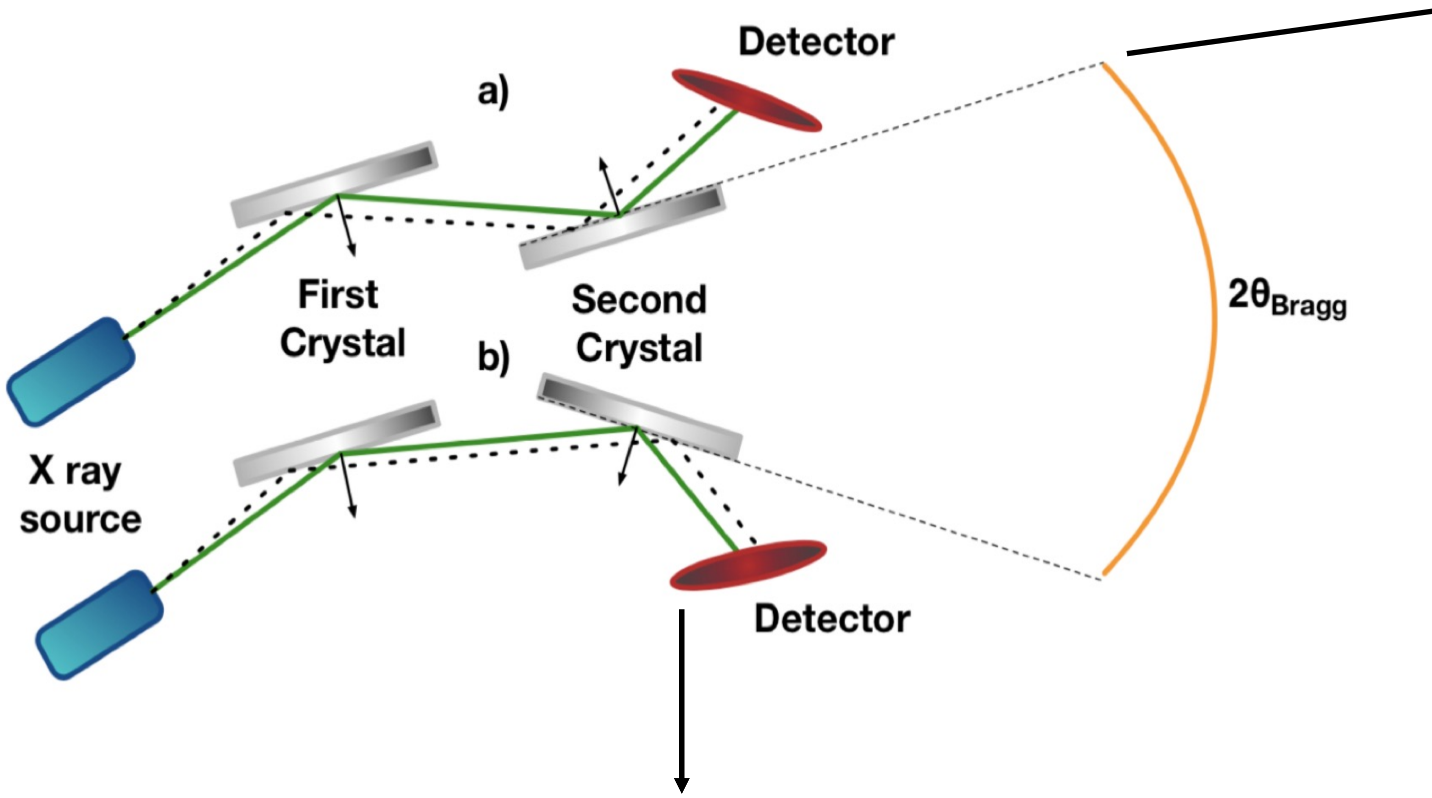


Ionisation process in the ECR source

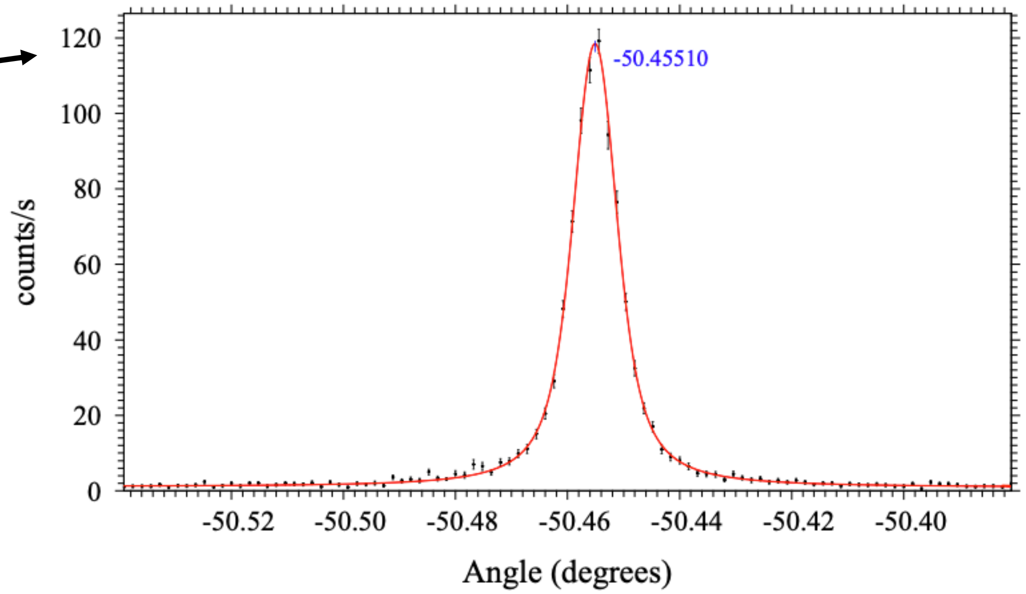
- Production of **H-like medium-Z** ions
- Systems with **open K-shell**

P. Amaro, S. Schlesser, M. Guerra, E. O. Le Bigot, J.-M. Isac, P. Travers, J. P. Santos, C. I. Szabo, A. Gumberidze, and P. Indelicato, Phys. Rev. Lett. **109**, 043005 (2012)
J. Machado, C. I. Szabo, J. P. Santos, P. Amaro, M. Guerra, A. Gumberidze, G. Bian, J. M. Isac, and P. Indelicato, Phys. Rev. A **97**, 032517 (2018).
J. Machado et al. Phys. Rev. A **101**, 062505 (2020)
J. Machado et al. Phys. Rev. A **107**, 032821 (2023)

Double Crystal Spectrometer (DCS)



Non dispersive Spectrum



Bragg's law:

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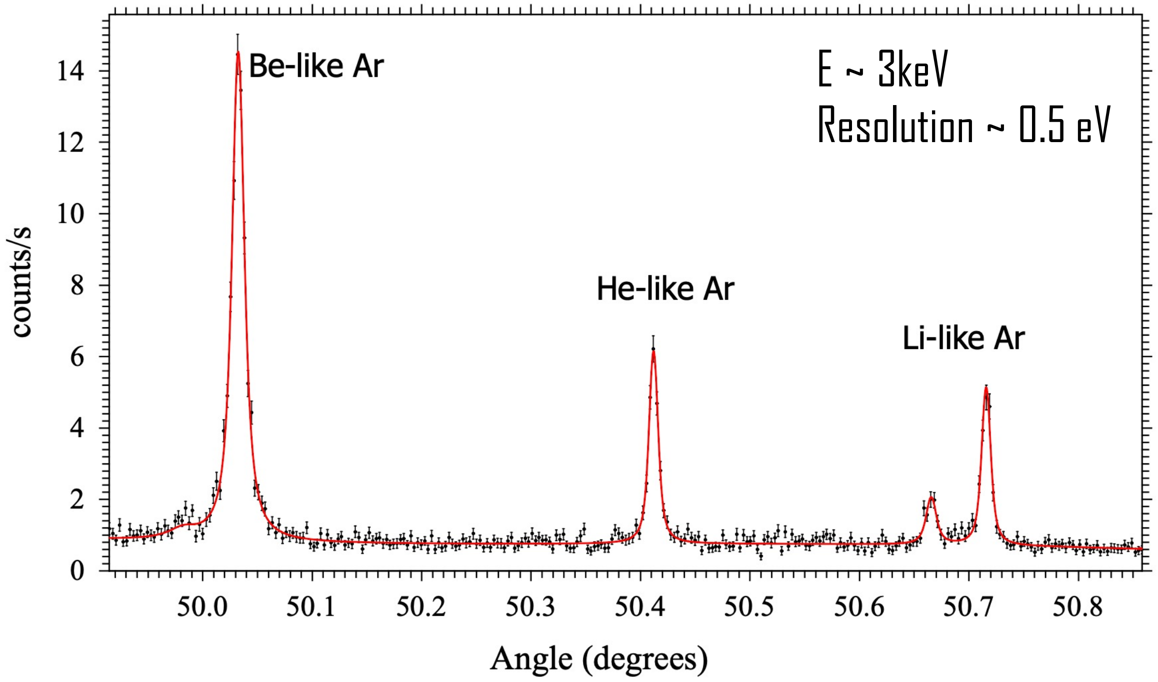
Dispersive Spectrum



E ~ 3keV
Resolution ~ 0.5 eV

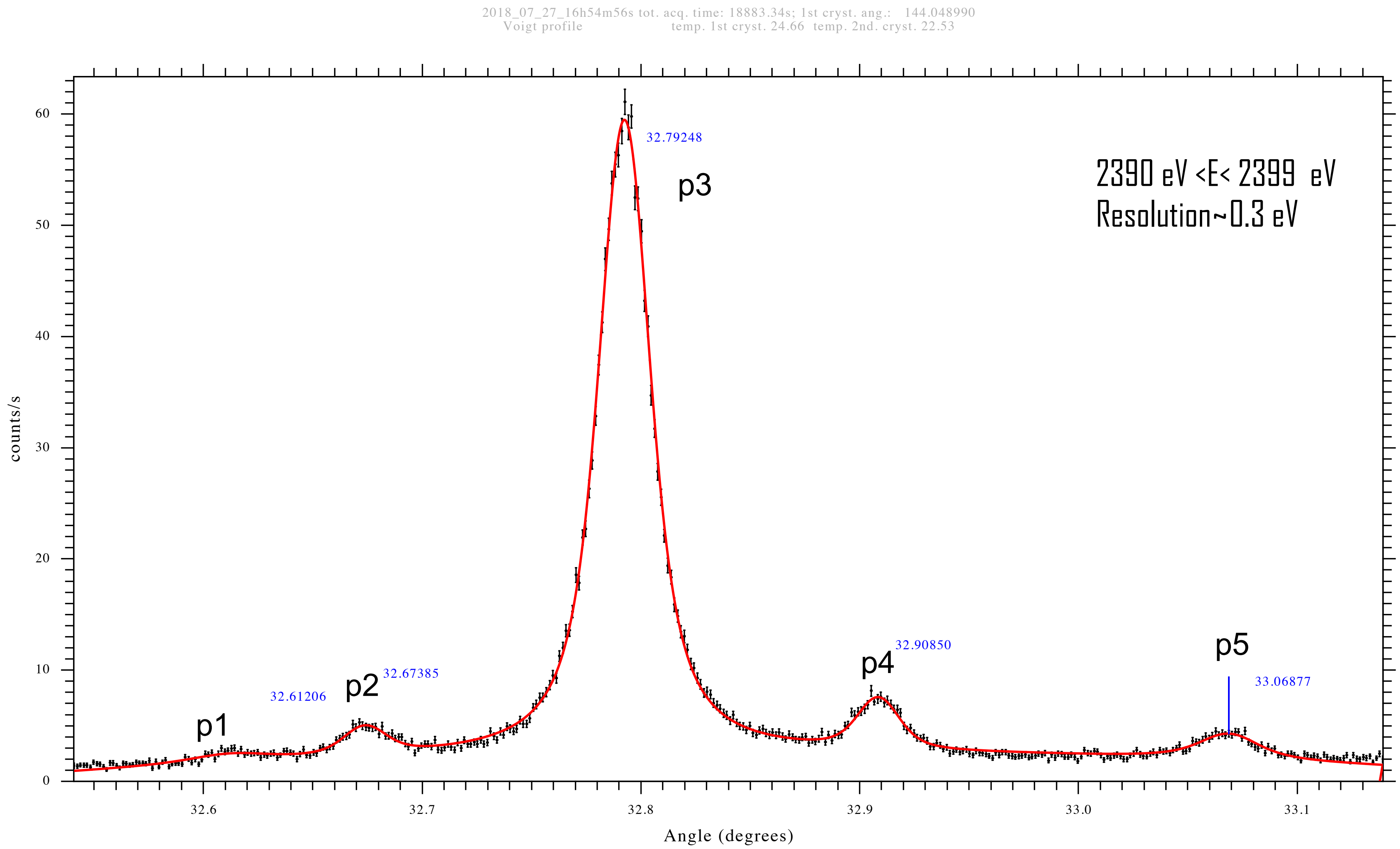
P. Amaro et al. / Rad. Phys. Chem. **98** (2014) 132–149

- Double Crystal Spectrometer
- Installed at the **ECR** source **SIMPA**
- **Reference free** measurement
- **Ppm** precision
- 1st crystal stays **fixed**
- Scan by **moving 2nd crystal**

B-like Argon and Sulfur

What kinds of transitions do we have?

Argon with 5 electrons



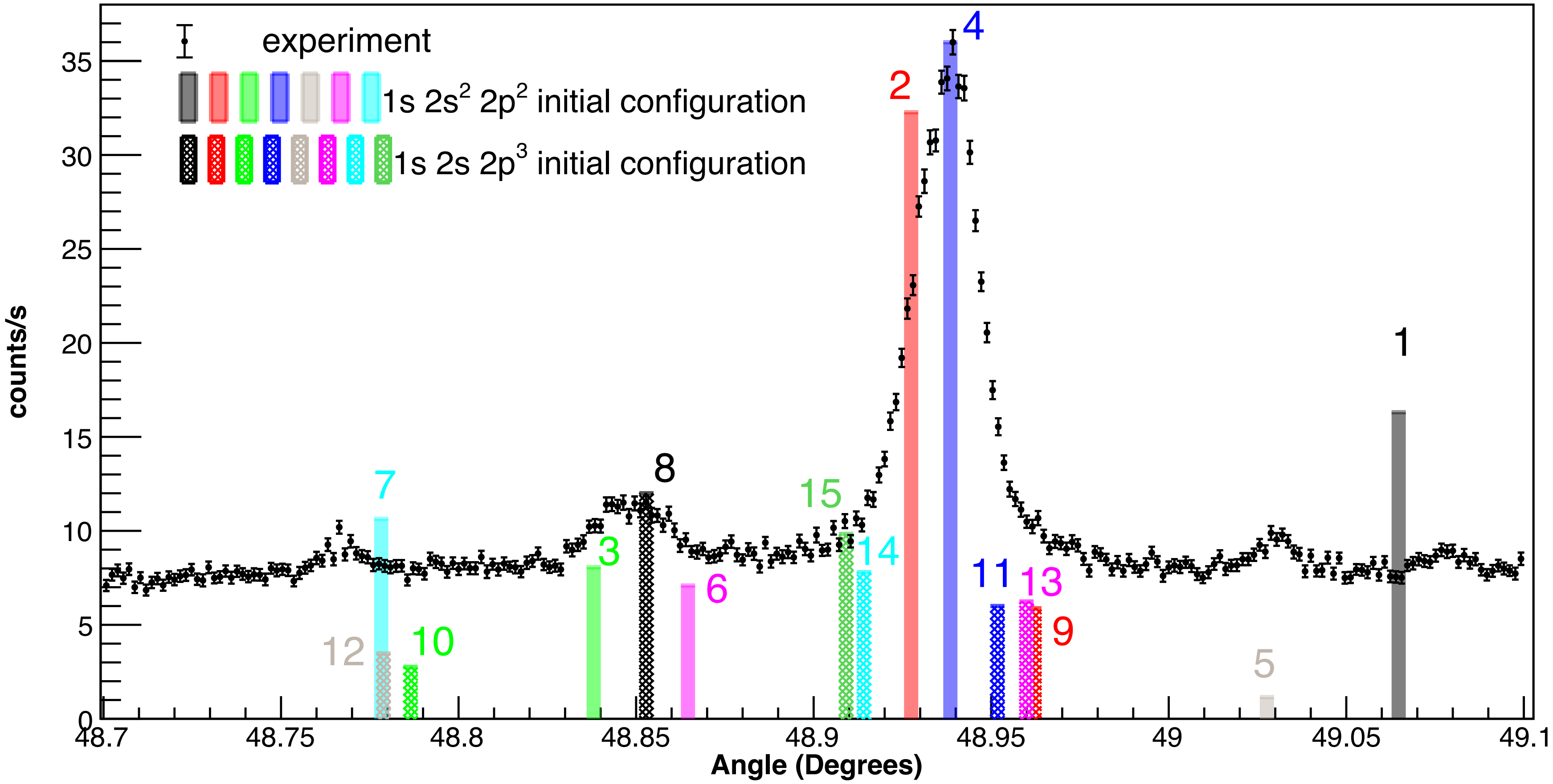
2390 eV <E< 2399 eV
Resolution~0.3 eV

Spectrum of B-like Sulfur from 2018

What kinds of transition inside those peaks?

Line number	Initial level		Final level		Transition energy [eV]	RT Yield
1	$1s\,2s^2\,2p^2$	$^2S_{1/2}$	$1s^2\,2s^2\,2p$	$^2P_{3/2}$	3069.60	0.184
2		$^2P_{1/2}$		$^1P_{3/2}$	3065.24	0.364
3		$^2P_{1/2}$		$^2P_{3/2}$	3062.41	0.091
4		$^2P_{3/2}$		$^2P_{3/2}$	3065.59	0.406
5		$^2P_{3/2}$		$^2P_{1/2}$	3068.42	0.026
6		$^2D_{3/2}$		$^2P_{1/2}$	3063.25	0.160
7		$^2D_{5/2}$		$^2P_{3/2}$	3060.52	0.120
8	$1s\,2s\,2p^3$	$^2P_{3/2}$	$1s^2\,2s\,2p^2$	$^2P_{3/2}$	3062.88	0.413
9		$^2P^{(1)}_{1/2}$		$^2D_{3/2}$	3066.34	0.201
10		$^2P^{(2)}_{1/2}$		$^2P_{1/2}$	3060.78	0.186
11		$^2P^{(1)}_{3/2}$		$^2D_{5/2}$	3066.01	0.139
12		$^2P^{(2)}_{3/2}$		$^2P_{3/2}$	3060.54	0.121
13		$^4P_{1/2}$		$^4P_{3/2}$	3066.27	0.214
14		$^4P_{3/2}$		$^4P_{5/2}$	3064.82	0.180
15		$^4P_{5/2}$		$^4P_{5/2}$	3064.66	0.225

Costa, A.M., et al., *Dirac-Fock transition energies and radiative and radiationless transition probabilities for Ar^{9+} to Ar^{16+}/ ion levels with K-shell holes.* Atomic Data and Nuclear Data Tables, 2001. **79**(2): p. 223-39.



Private Communication from Paul Indelicato (2017)

- Boron-like Sulfur and Argon were measured thanks to the DCS.
- Complex spectrum with many lines
- Need to understand the spectra

Bayesian analysis

- The higher the evidence, the higher the probability for the model to describe
- Favor models with less number of parameters
- Use of nested_fit, a nested sampling algorithm from Martino Trassinelli *et al.*
- Use of flat priors

$$\overset{\text{Model probability}}{P(M|\{x_i,y_i\},I)} \propto \overset{\text{Bayesian evidence}}{P(\{x_i,y_i\}|M,I)} \times \overset{\text{Priors on the models}}{P(M|I)}$$

$$\| $$

$$\int \underset{\uparrow\ \text{Likelihood}}{P(\{x_i,y_i\}|\boldsymbol{\theta},M,I)} \times \underset{\uparrow\ \text{Parameter priors (it defines the integration volume)}}{P(\boldsymbol{\theta}|M,I)}\, d^n\boldsymbol{\theta}$$

Model each peak with Voigt Profile(s) → Compare the evidences for different numbers of contributions

$$V(x) \propto \int_{-\infty}^{+\infty} \mathrm{e}^{-a\cdot t^2} \times \frac{1}{b+(x-x_0-t)^2}\,\mathrm{d}t$$

$$G(x;\sigma) \equiv \frac{e^{-x^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}}$$: Gaussian Broadening

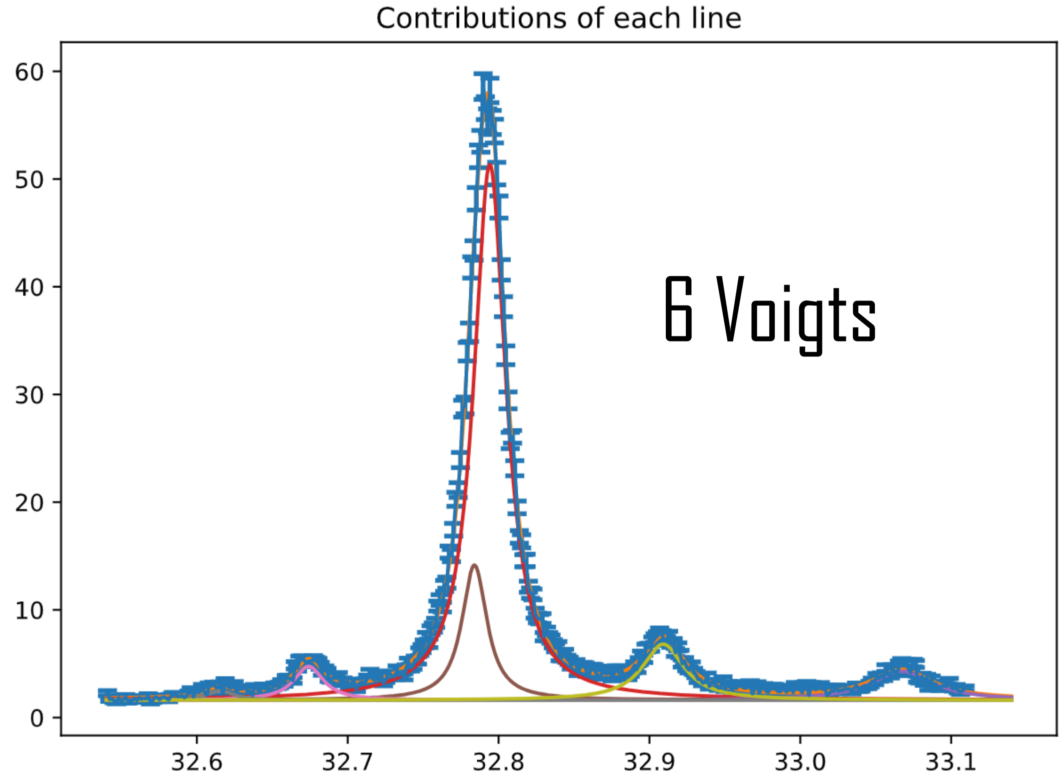
$$L(x;\gamma) \equiv \frac{\gamma}{\pi(x^2+\gamma^2)}$$: Natural line profile

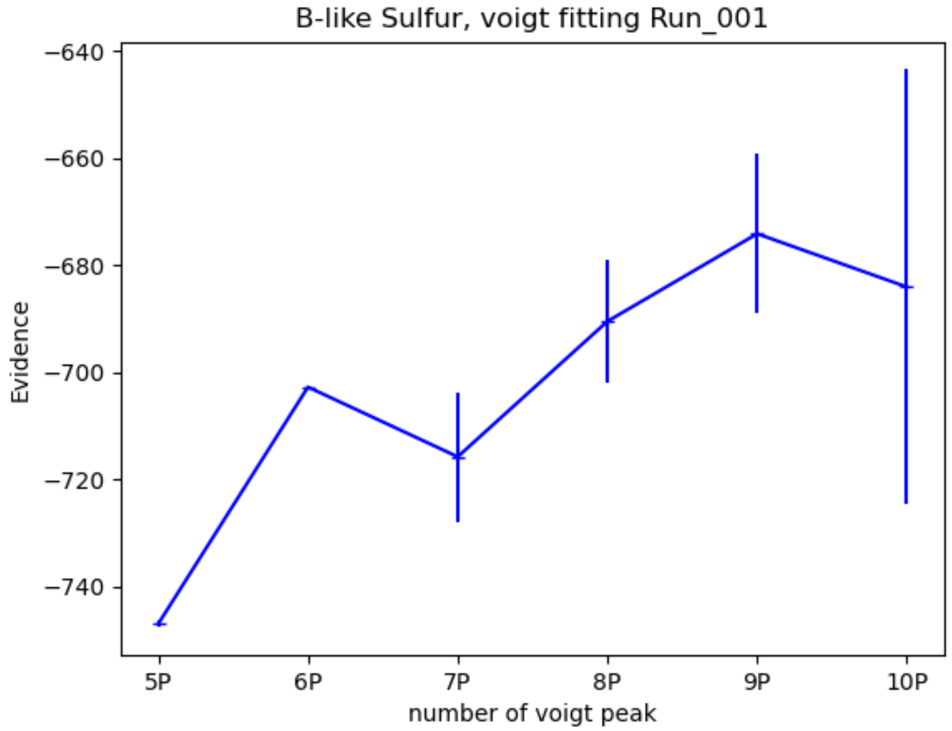
Model=$\sum Voigt(Amp,\theta,\gamma,\sigma)$

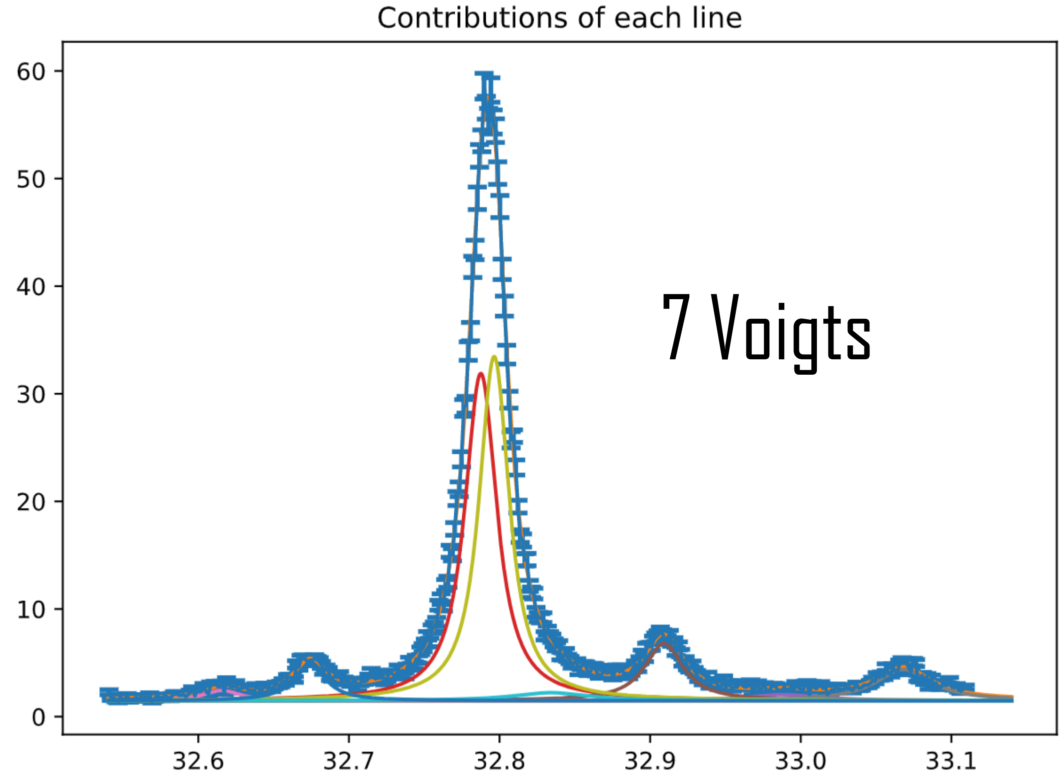
5 electrons (Boron-like) sulfur

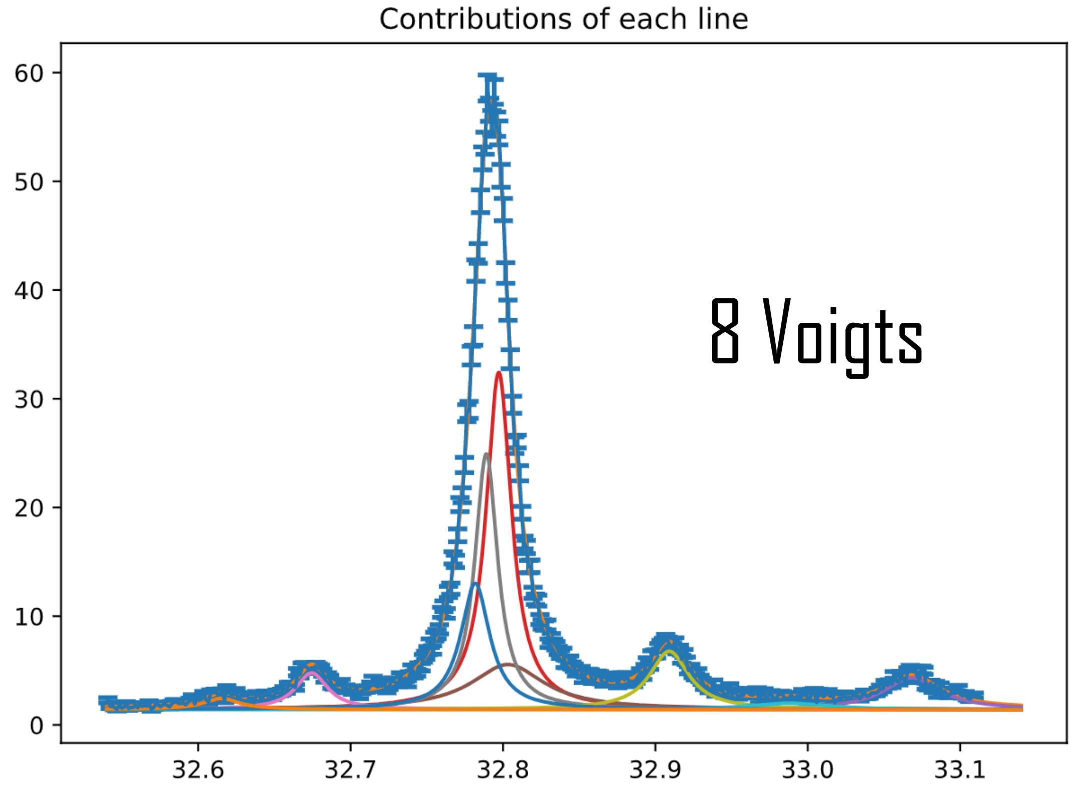
Atomic transition or no atomic transition, that is the question

Naive fitting is hard


Contributions of each line

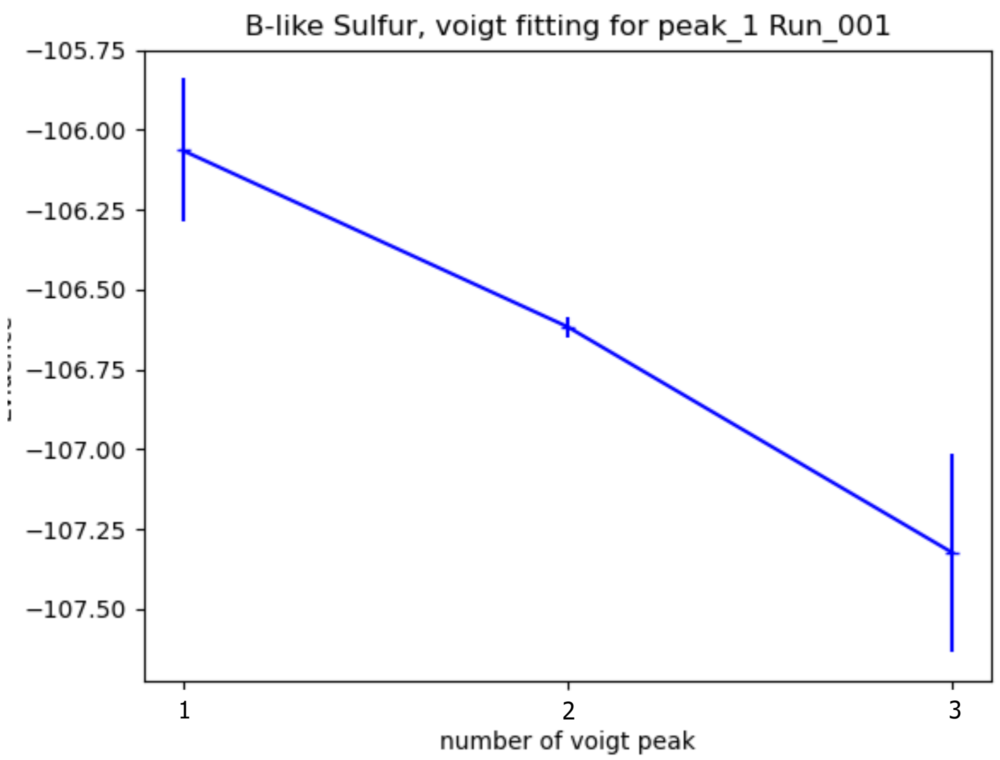

B-like Sulfur, voigt fitting Run_001

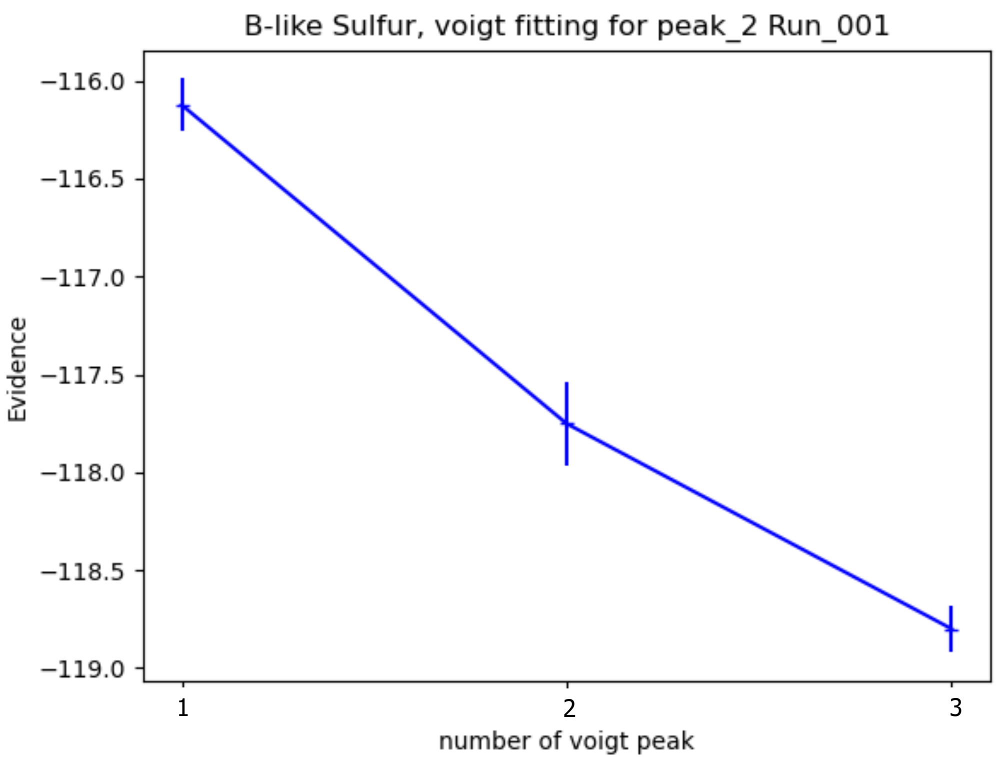

Contributions of each line

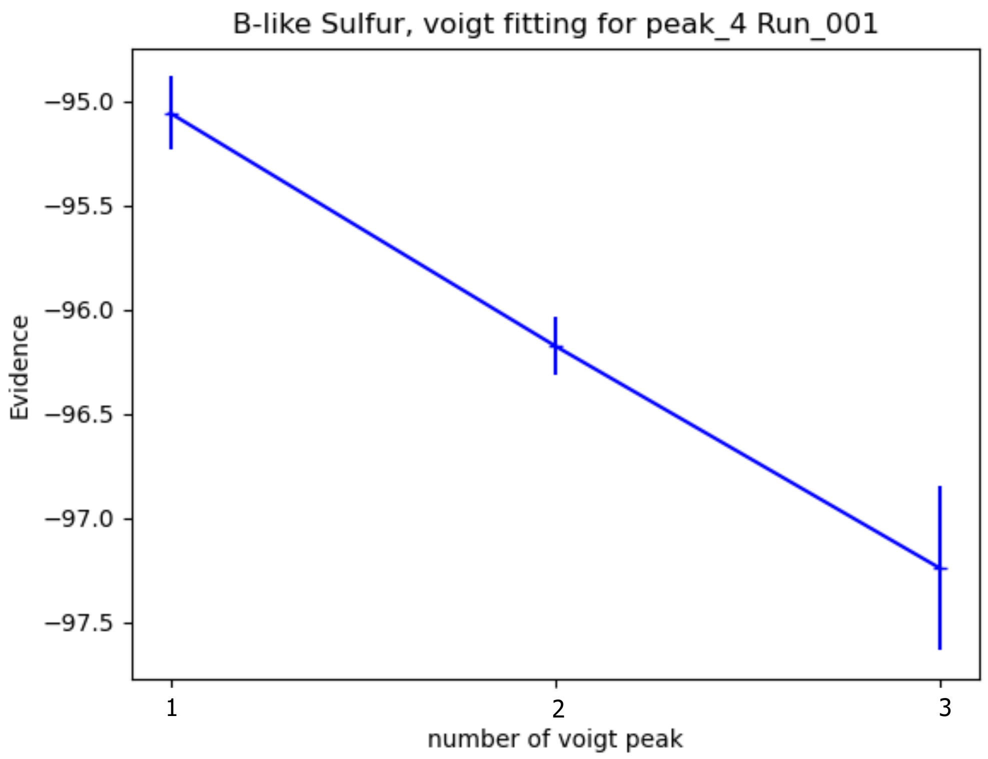

Contributions of each line

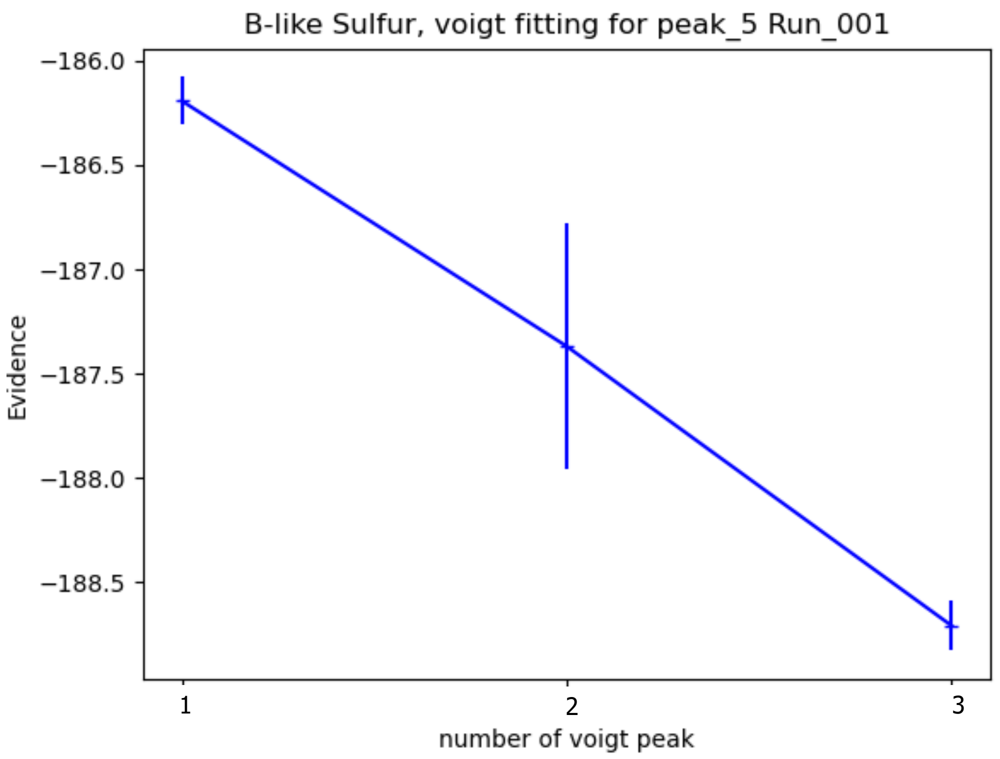
Model=$\sum Voigt(Amp,\theta,\gamma,\sigma)$

Cutting peak per peak helps!





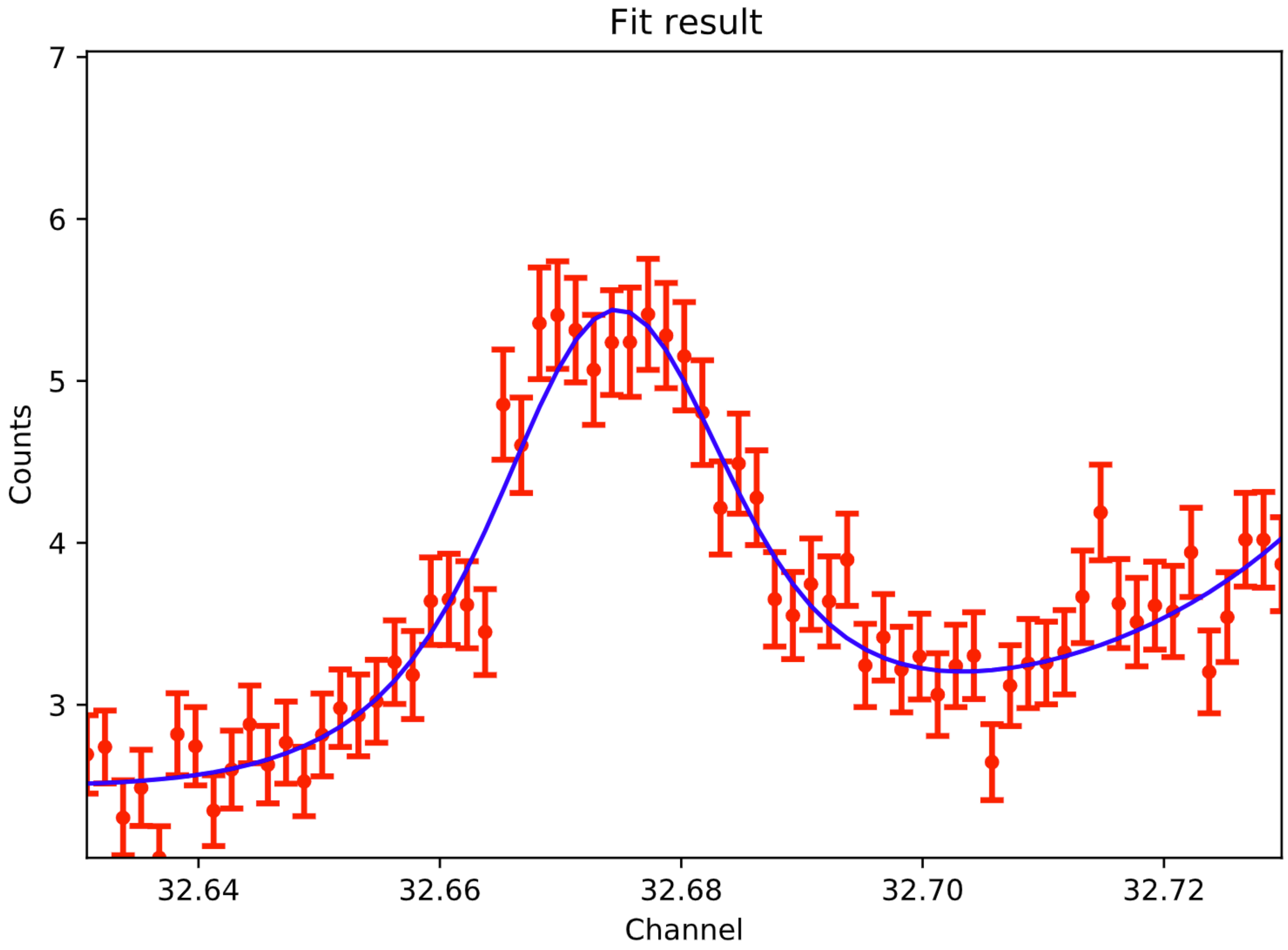




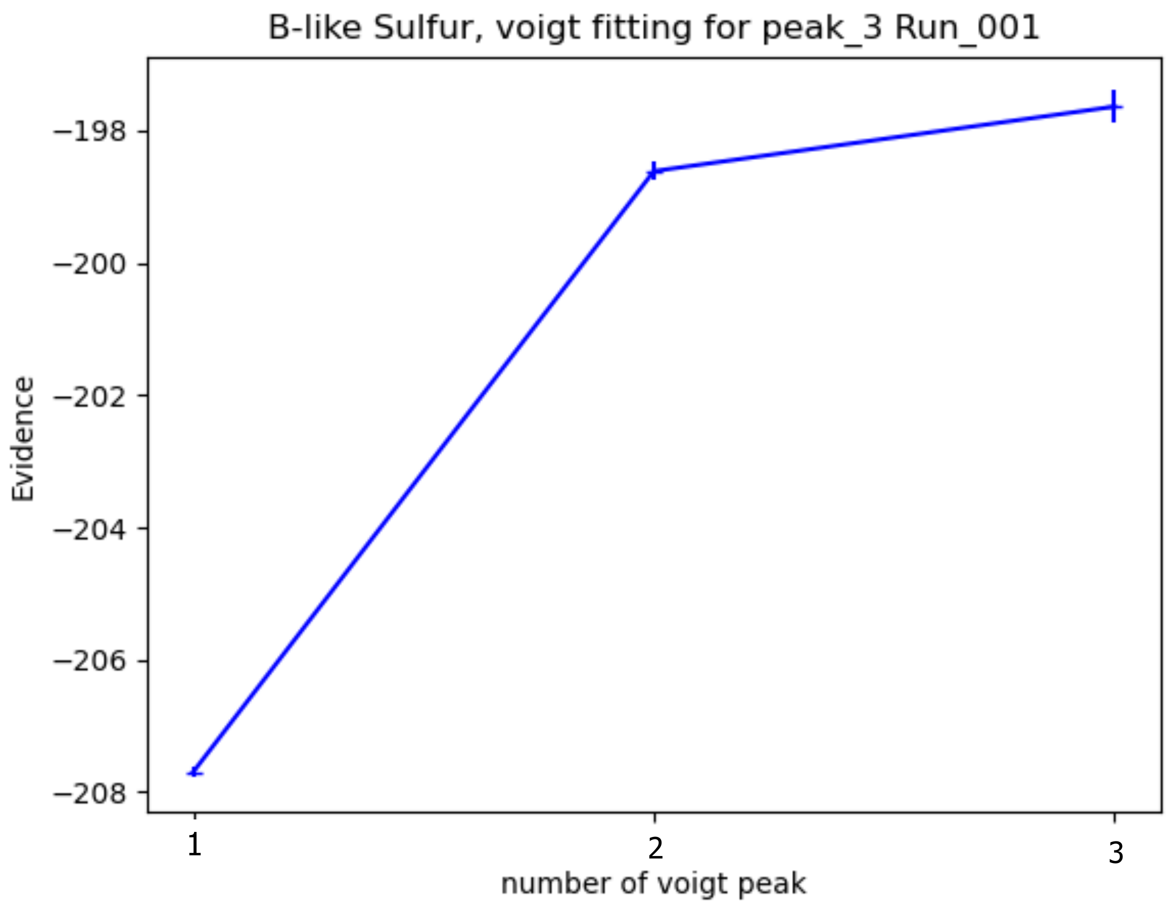
Model=$\sum Voigt(Amp, \theta, \gamma, \sigma)$

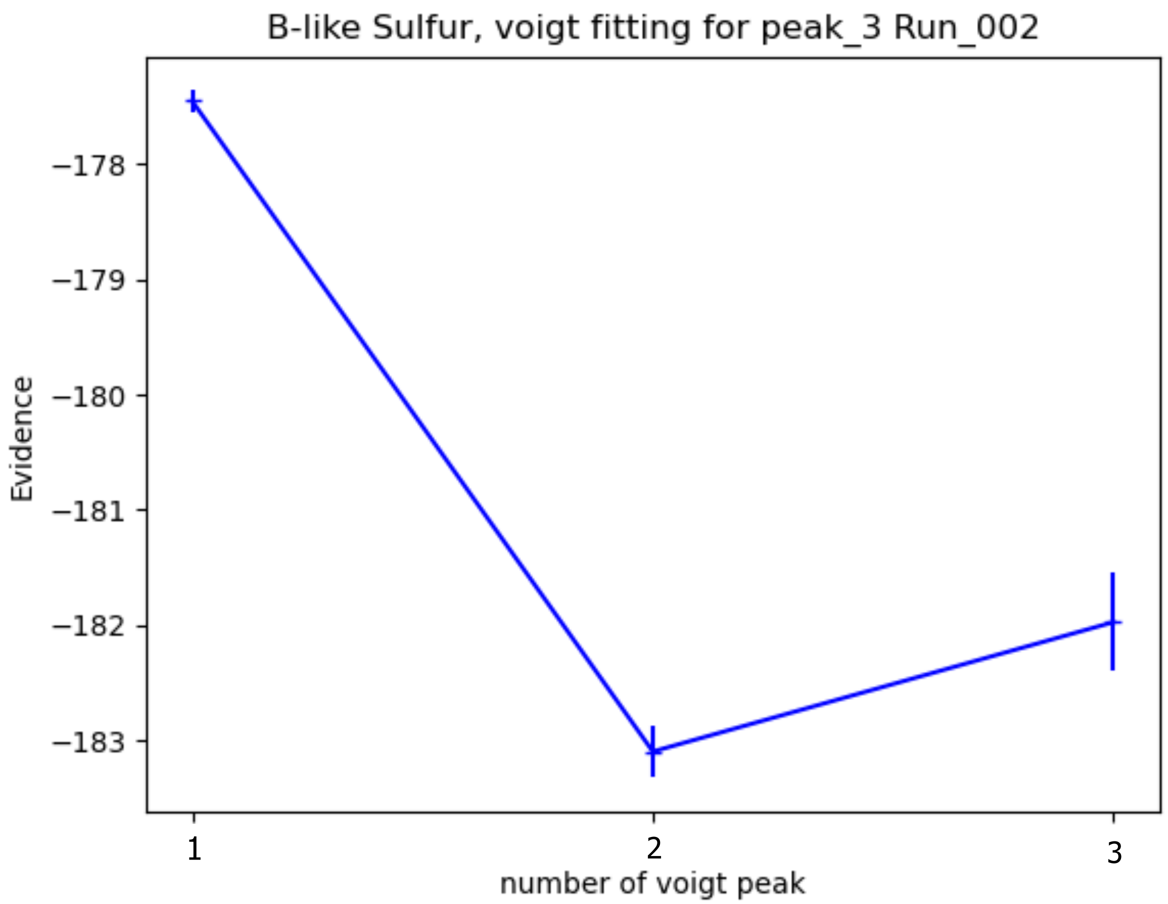
Example of the best fit for the first peak

1 Voigt model



Peak 3

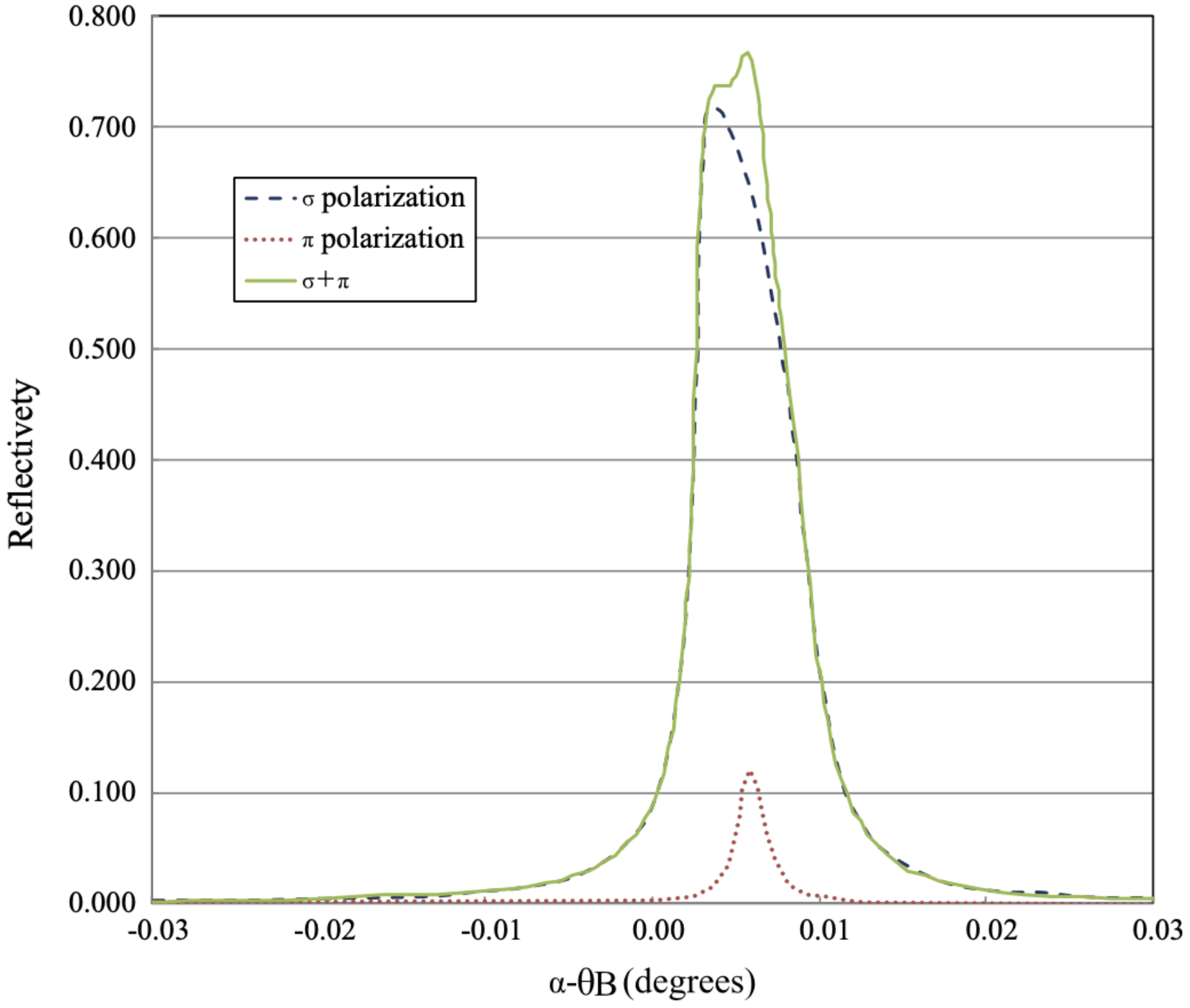




Model=$\sum Voigt(Amp,\theta,\gamma,\sigma)$

Peak with high statistics: Is Voigt profile the right model to study this peak?

Spectrometer

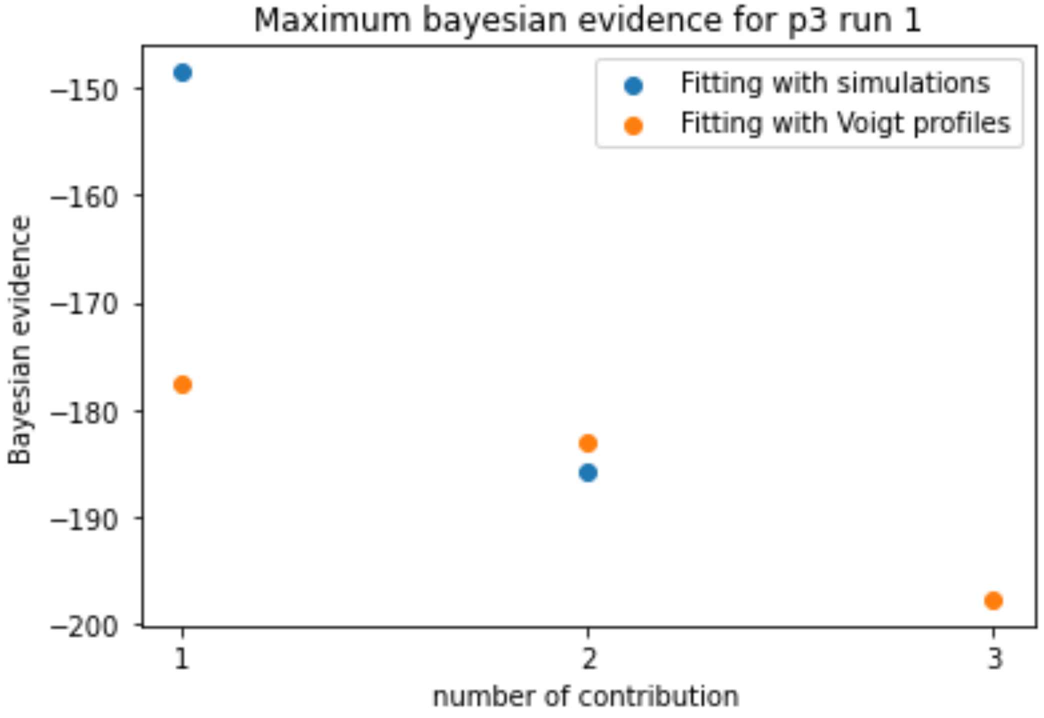


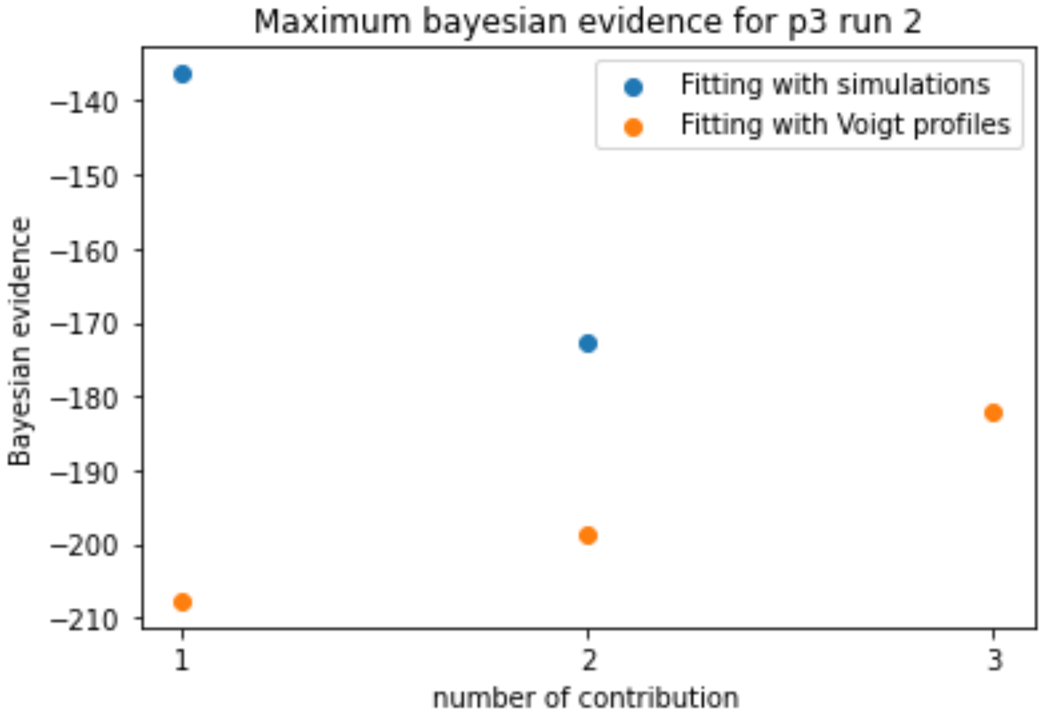
Rocking curve around θ_{Bragg}

- Reflectivity of the crystal depends on the crystal
- Dispersion changes with the energy
- Can be interpolated and convoluted with the profile
- Real doppler broadening can be taken into account

J. Machado, C. I. Szabo, J. P. Santos, P. Amaro, M. Guerra, A. Gumberidze, G. Bian, J. M. Isac, and P. Indelicato, Phys. Rev. A **97**, 032517 (2018).
J. Machado, N. Paul, G. Soum-Sidikov, et al, Phys. Rev. A **107**, 032821 (2023).

Peak 3 with interpolation and neighbours

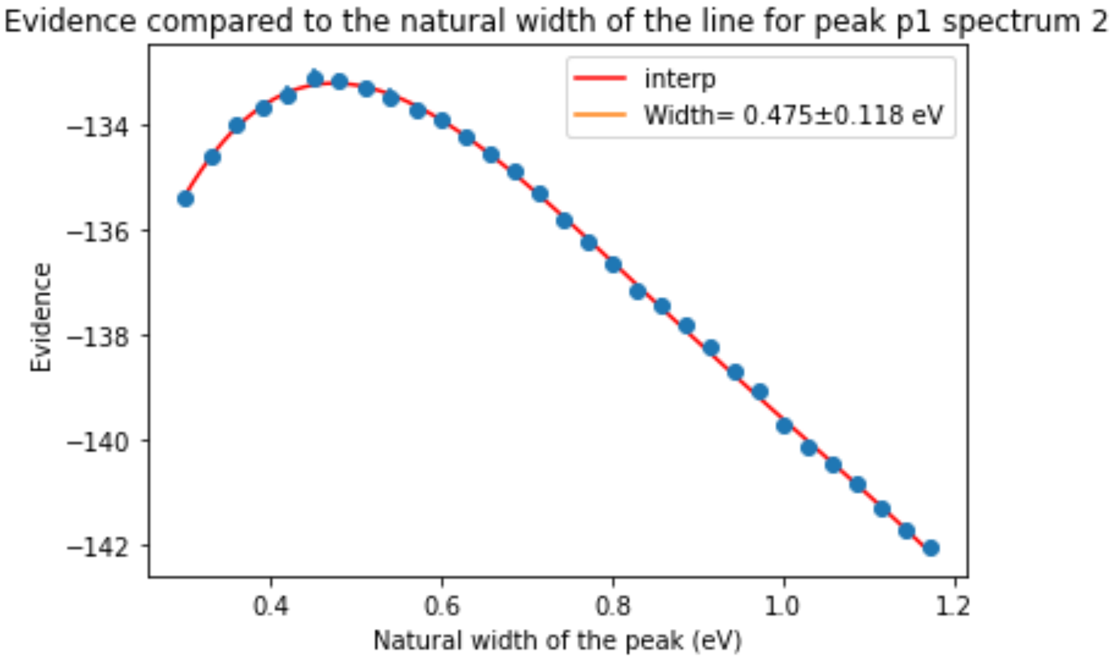


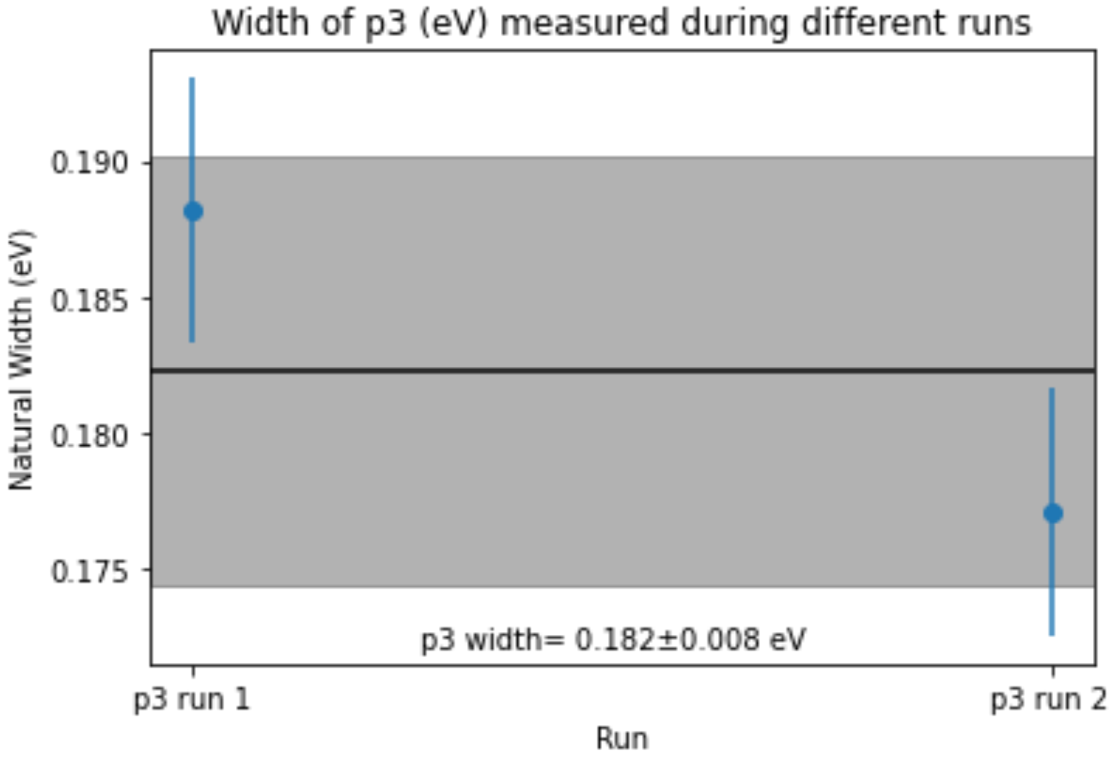


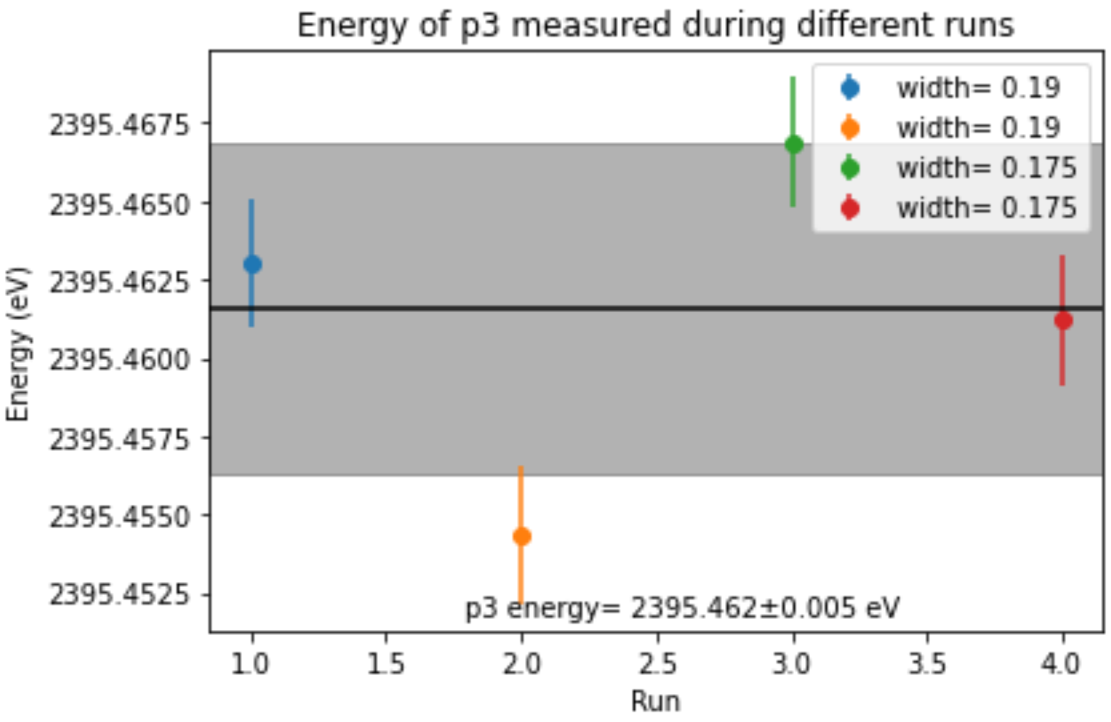
- By using simulations, we get a more precise lineshape of the spectrum
- BE is better with simulations than Voigts
- BE tends to show the only 1 peak is present
- Error bars are within the symbols

Model=$\sum Simu(Amp, \theta, \sigma)$

Determination of the width


Evidence compared to the natural width of the line for peak p1 spectrum 2


Width of p3 (eV) measured during different runs

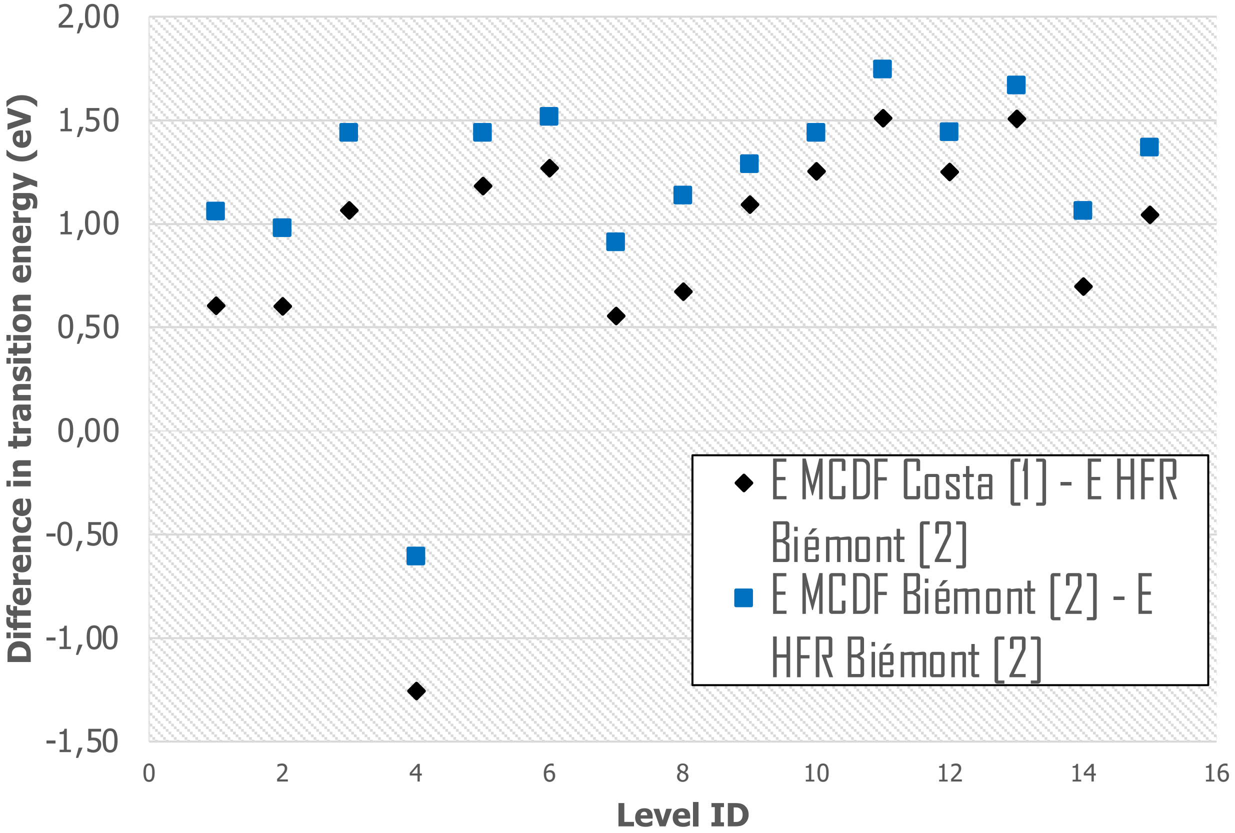

Energy of p3 measured during different runs

- The evidence is fitted with a 4th order polynomial
- The maximum of the evidence gives the width
- Maximum of evidence -0.9 gives the uncertainties at ~±1.9σ
- Difference in angle between the simulation and spectra gives the energy

Comparison with the theory

Line Number	Initial Level	Final Level	MCDF [1]	HFR [2]	MCDF [2]
1	$1s2s^22p^2\ ^2D_{5/2}$	$1s^22s^22p\ ^2P_{3/2}$	3060, 53	3059, 92	3060, 98
2	$1s2s^22p^2\ ^2P_{1/2}$	$1s^22s^22p\ ^2P_{3/2}$	3062, 41	3061, 81	3062, 79
3	$1s2s^22p^2\ ^2D_{3/2}$	$1s^22s^22p\ ^2P_{1/2}$	3063, 25	3062, 19	3063, 63
4	$1s2s2p^3\ ^2S_{1/2}$	$1s^22s2p^2\ ^2P_{1/2}$	3064, 19	3065, 44	3064, 84
5	$1s2s2p^3\ ^4P_{5/2}$	$1s^22s2p^2\ ^4P_{5/2}$	3064, 66	3063, 48	3064, 91
6	$1s2s2p^3\ ^4P_{3/2}$	$1s^22s2p^2\ ^4P_{5/2}$	3064, 82	3063, 55	3065, 07
7	$1s2s^22p^2\ ^2P_{1/2}$	$1s^22s^22p\ ^2P_{1/2}$	3065, 24	3064, 69	3065, 60
8	$1s2s^22p^2\ ^2P_{3/2}$	$1s^22s^22p\ ^2P_{3/2}$	3065, 59	3064, 91	3066, 05
9	$1s2s2p^3\ ^4P_{5/2}$	$1s^22s2p^2\ ^4P_{3/2}$	3066, 08	3064, 99	3066, 28
10	$1s2s2p^3\ ^4P_{3/2}$	$1s^22s2p^2\ ^4P_{3/2}$	3066, 24	3064, 99	3066, 43
11	$1s2s2p^3\ ^4P_{1/2}$	$1s^22s2p^2\ ^4P_{3/2}$	3066, 27	3064, 76	3066, 51
12	$1s2s2p^3\ ^4P_{3/2}$	$1s^22s2p^2\ ^4P_{1/2}$	3067, 30	3066, 05	3067, 49
13	$1s2s2p^3\ ^4P_{1/2}$	$1s^22s2p^2\ ^4P_{1/2}$	3067, 33	3065, 82	3067, 49
14	$1s2s^22p^2\ ^2P_{3/2}$	$1s^22s^22p^1\ ^2P_{1/2}$	3068, 42	3067, 72	3068, 78
15	$1s2s^22p^2\ ^2S_{1/2}$	$1s^22s^22p^1\ ^2P_{3/2}$	3069, 60	3068, 56	3069, 92

Theoretical energies for transitions in B-like Ar from
[1] A.M. Costa *et al*, At. At.Data Nucl. Data Tables, 2001. **79**(2)
[2] E. Biémont *et al*, Phys. Scr., 2000. **61**(555)



Comparison of energies between calculation from Costa *et al* (2001) and Biémont *et al* (2000)

- Theoretical papers are giving energies with less than 1eV of agreement
- No treatment of correlations
- Correlations can shuffle all the energies by more than 2eV
- It is not possible to identify the lines with current calculations

P. Indelicato, *J. Phys. B: At. Mol. Opt. Phys.* **52** 232001 (2019)

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4	$1s2s2p^3\ ^2S_{1/2}$	$1s^22s2p^2\ ^2P_{1/2}$	3064,19	3065,44	3064,84
5	$1s2s2p^3\ ^4P_{5/2}$	$1s^22s2p^2\ ^4P_{5/2}$	3064,66	3063,48	3064,91
6	$1s2s2p^3\ ^4P_{3/2}$	$1s^22s2p^2\ ^4P_{5/2}$	3064,82	3063,55	3065,07
7	$1s2s^22p^2\ ^2P_{1/2}$	$1s^22s^22p\ ^2P_{1/2}$	3065,24	3064,69	3065,60
8	$1s2s^22p^2\ ^2P_{3/2}$	$1s^22s^22p\ ^2P_{3/2}$	3065,59	3064,91	3066,05
9	$1s2s2p^3\ ^4P_{5/2}$	$1s^22s2p^2\ ^4P_{3/2}$	3066,08	3064,99	3066,28
10	$1s2s2p^3\ ^4P_{3/2}$	$1s^22s2p^2\ ^4P_{3/2}$	3066,24	3064,99	3066,43
11	$1s2s2p^3\ ^4P_{1/2}$	$1s^22s2p^2\ ^4P_{3/2}$	3066,27	3064,76	3066,51
12	$1s2s2p^3\ ^4P_{3/2}$	$1s^22s2p^2\ ^4P_{1/2}$	3067,30	3066,05	3067,49
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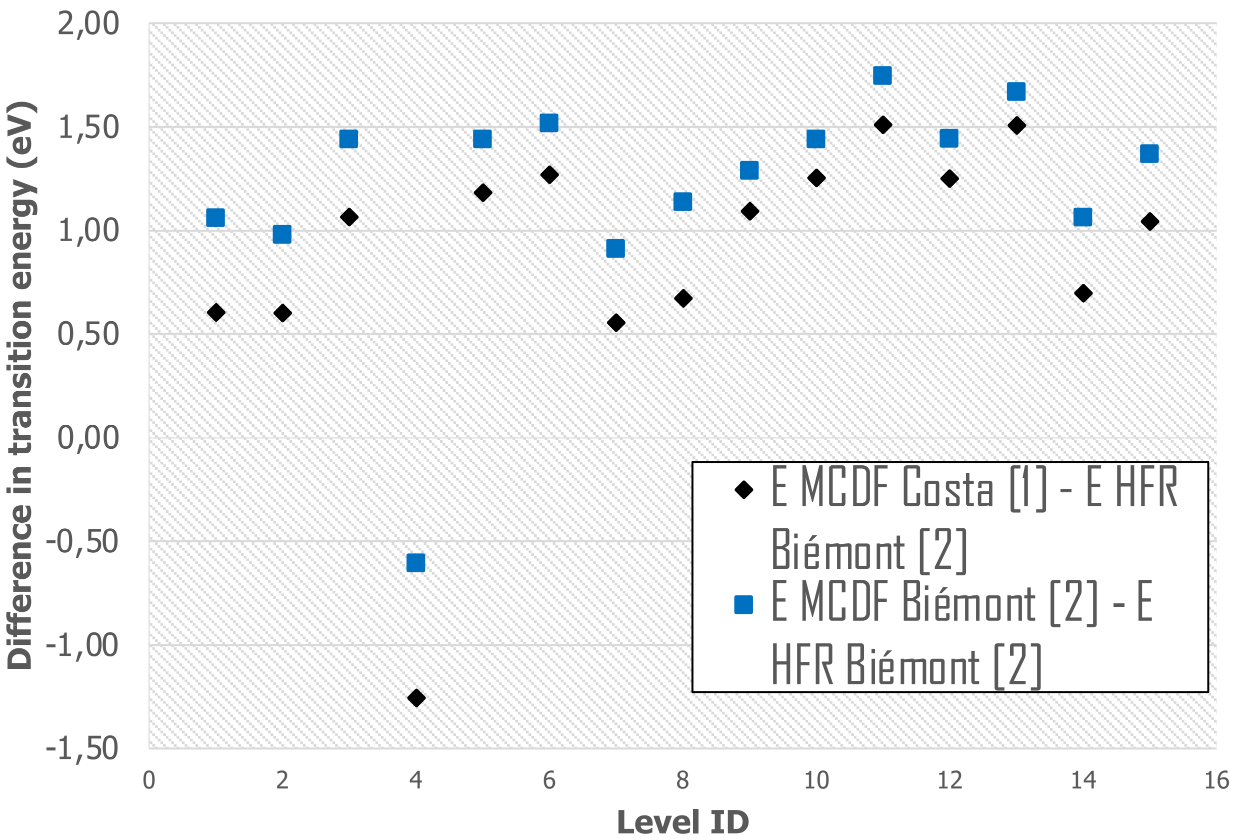

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New calculations are currently performed by the group!

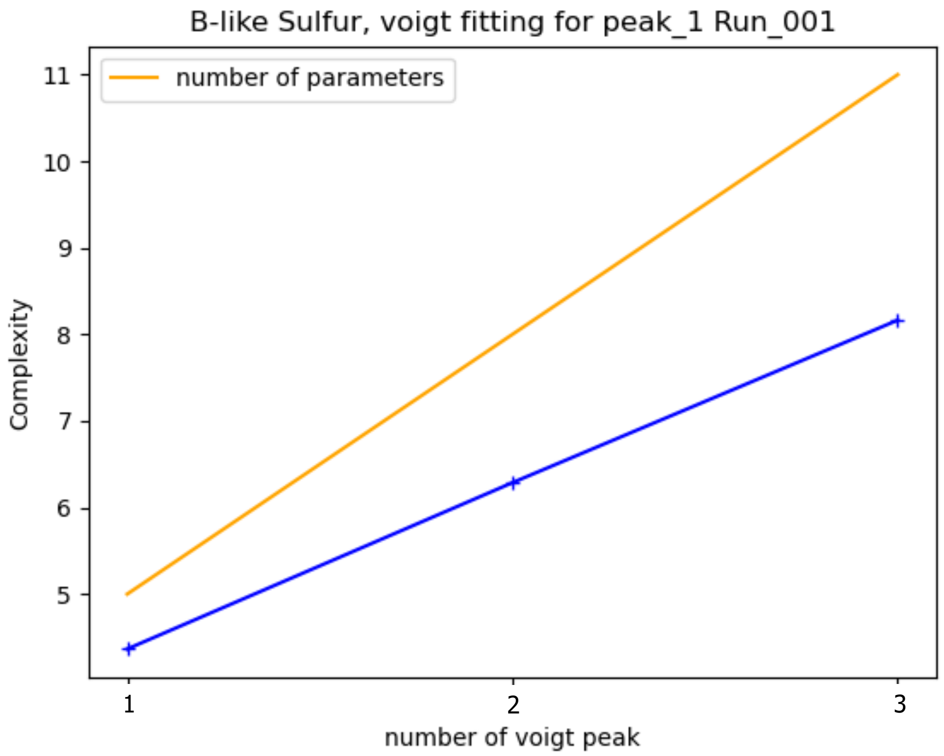
P. Indelicato, *J. Phys. B: At. Mol. Opt. Phys.* **52** 232001 (2019)

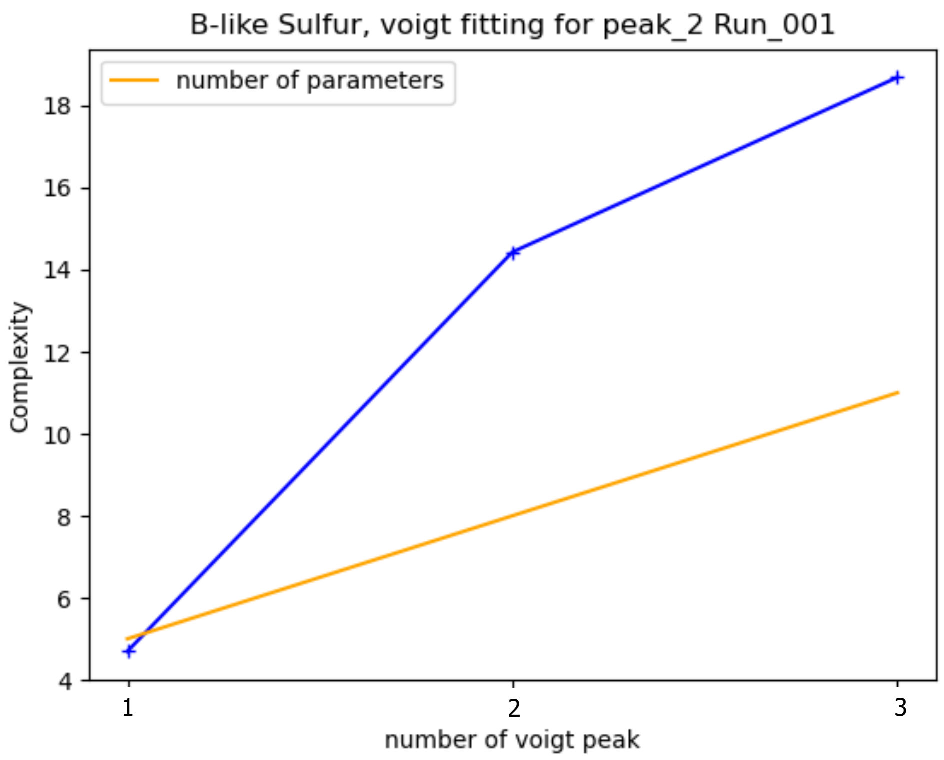
Conclusion

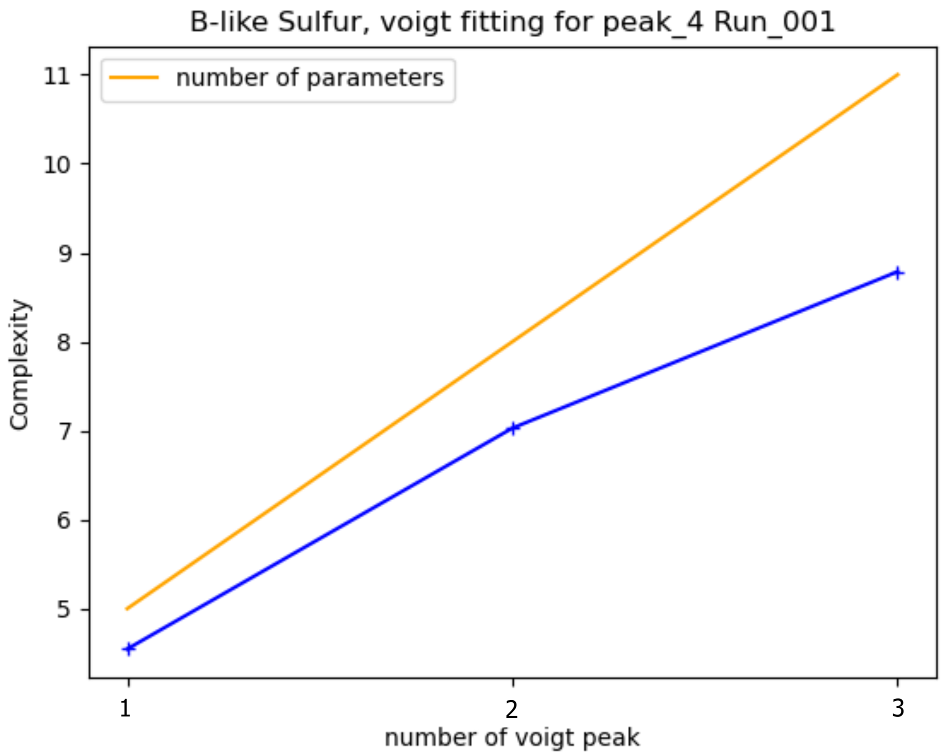
- BE allows to compare efficiently different models, and to unveil (or not!) hidden contributions
- We find only one atomic line per visible peak for B-like Sulfur. We were also able to determine the width of each contribution
- We are also investigating the relative amplitudes of each peak to help us identify the atomic rays
- Theory is still not accurate enough to provide indentification
- Theoretical work is ongoing by the group to help for the identification of the lines
- Next: Analysing Argon, and make 2d splines of simulations to make it become a parameter
- Next: Take into account the whole spectrum

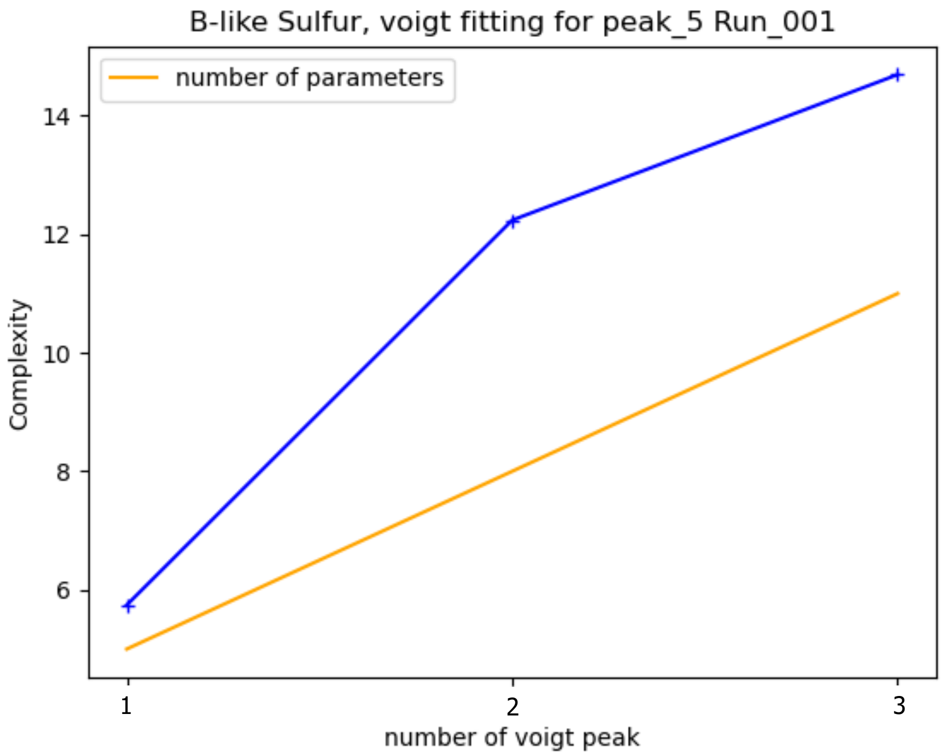
Thank You!

Bayesian complexity


B-like Sulfur, voigt fitting for peak_1 Run_001


B-like Sulfur, voigt fitting for peak_2 Run_001


B-like Sulfur, voigt fitting for peak_4 Run_001


B-like Sulfur, voigt fitting for peak_5 Run_001

Model=$\sum Voigt(Amp,\theta,\gamma,\sigma)$

Bayesian Complexity