Challenges in the analysis of the spectra of tritium-containing molecules

E. Pawelec[1], S. Brezinsek[2], M. Groth[3], A. Meigs[4], S. Menmuir[4], B. Thomas[4], D. Douai[5], G. Sergienko[2] and JET Contributors[*]

[1]Institute of Physics, University of Opole, Opole, Poland; [2]Forschungszentrum Jülich GmbH, EURATOM Association, Jülich, Germany; [3]Aalto University, Espoo, Finland; [4]Culham Science Centre, UK Atomic Energy Authority, Abingdon, UK; [5]CEA, IRFM, Saint-Paul-Lez-Durance, France;
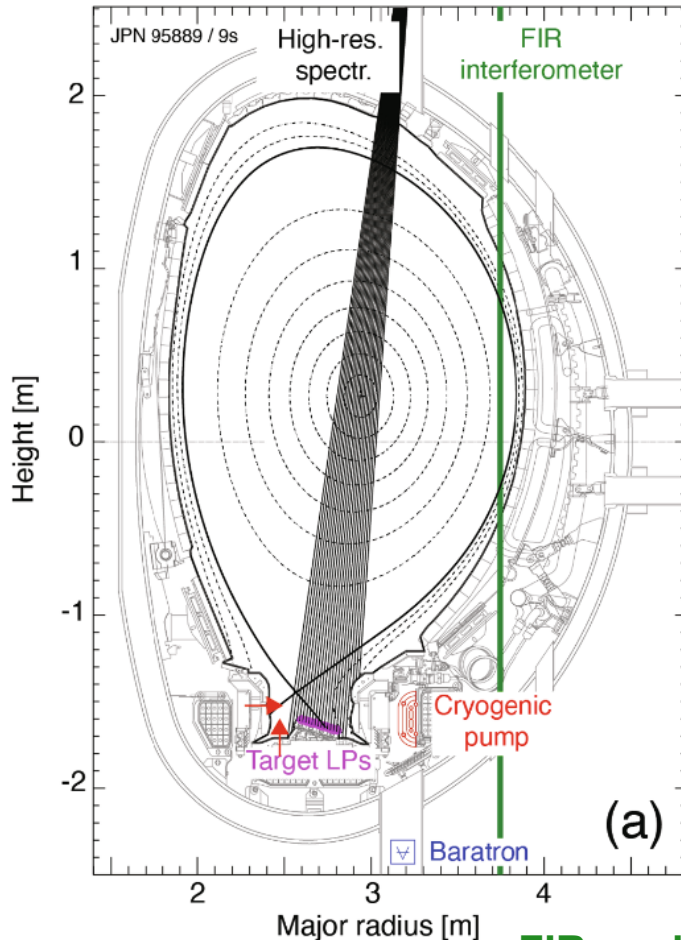
*See the author list of Mailloux et al, Nucl. Fusion 62 (2022) 042026

Main points

- Case study – density scan from attached to detached conditions

- Rotationally resolved spectrum – analysis

    - $D_2 + T_2$: DT molecule parameters

    - T_2: rotational temperature estimation

- Estimated total T_2 intensity

    - Spatial distribution in the divertor

    - Correlations with intensity of the 0-0 band, ion flux etc.

JET Diagnostics

JET divertor visible spectroscopy

Tunable high resolution mirror-link spectrometers with spatial resolution (22 tracks) for measuring hydrogenic lines and continuum background (for N_e and T_e calculation) and Fulcher bands simultaneously
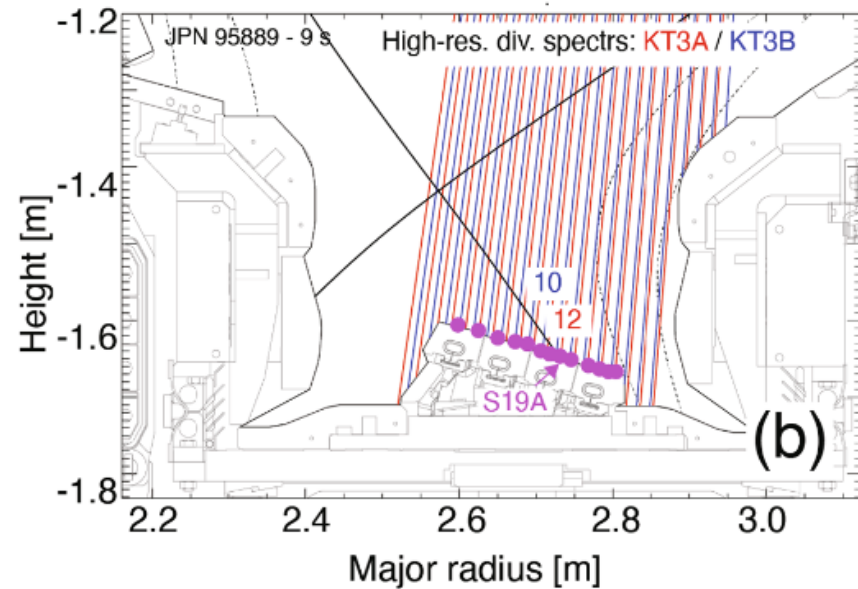
Langmuir Probes – ion flux to the surface
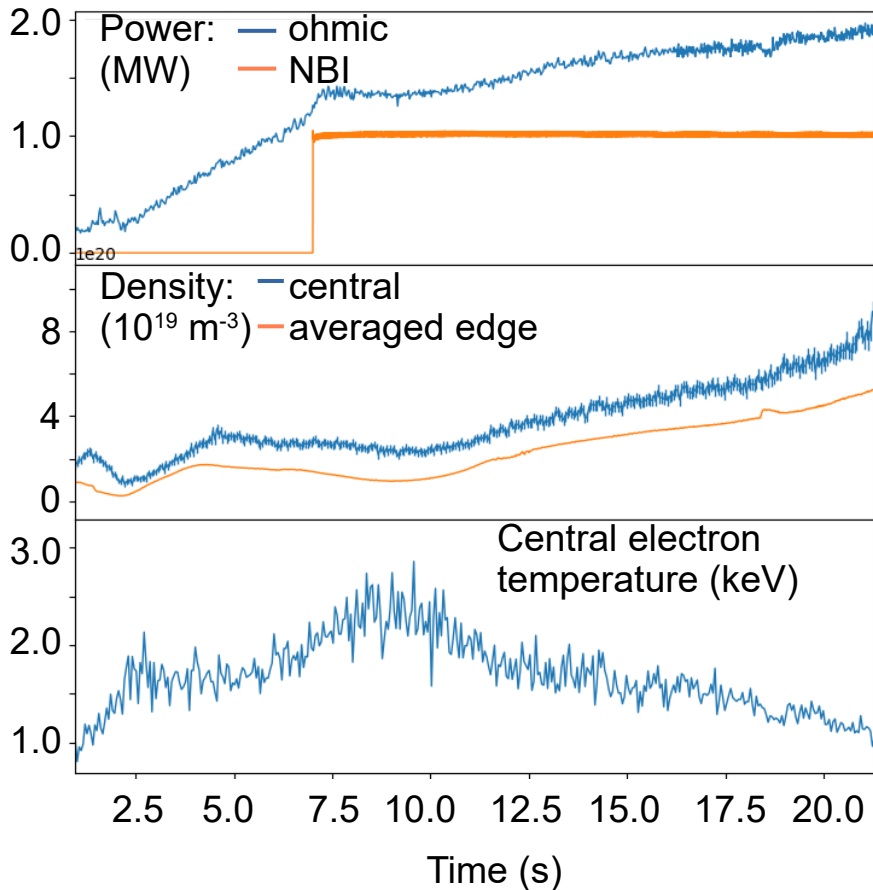
FIR – edge plasma density

Groth et al, **NME** *34 (2023) 101345*
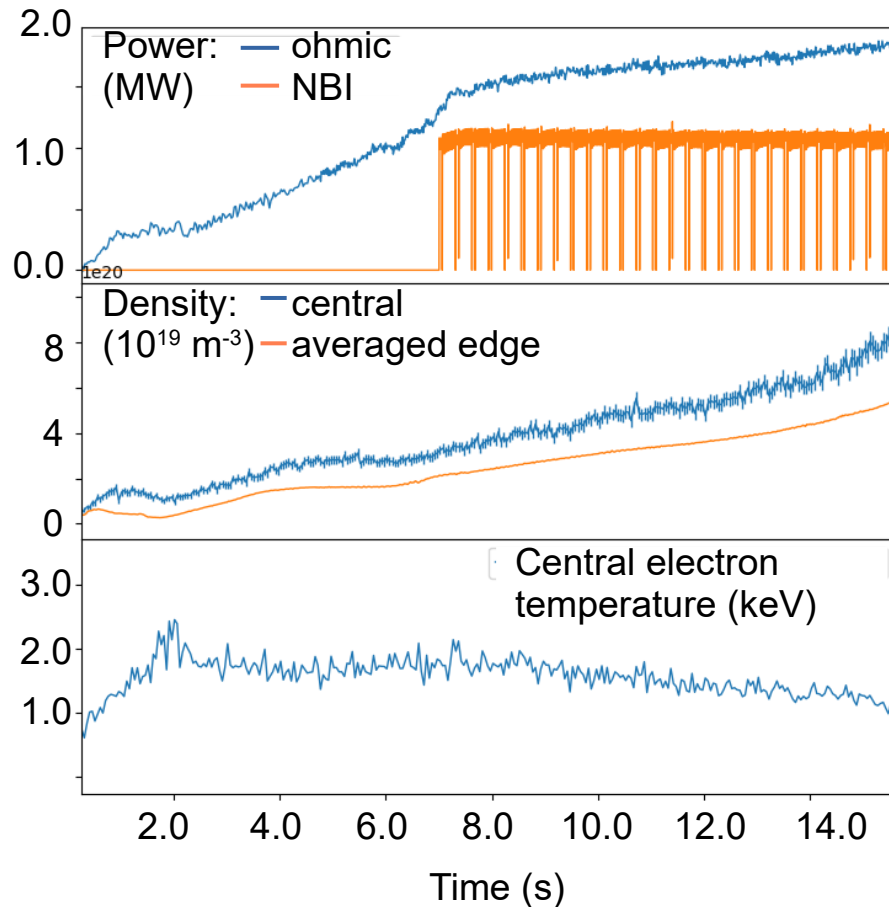
Analyzed pulses

Density scans in T (#100166)

$B_t = 2.51T$ $I_p = 2.5$ MA

and D(40%) T(60%) (#99433)

$B_t = 2.5T$ $I_p = 2.45$ MA
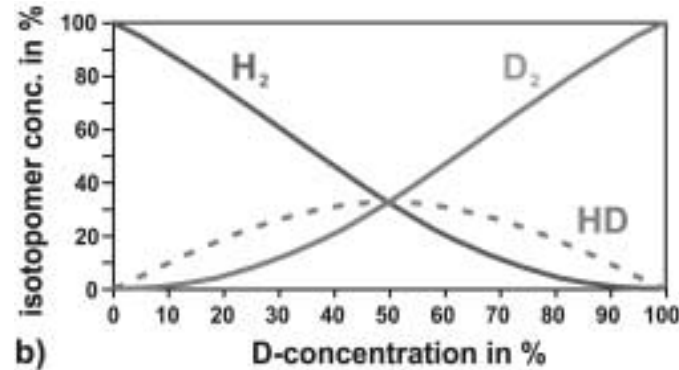

*Groth et al, **NME** 34 (2023) 101345*

Resolved spectra analysis
(DT, T$_2$)

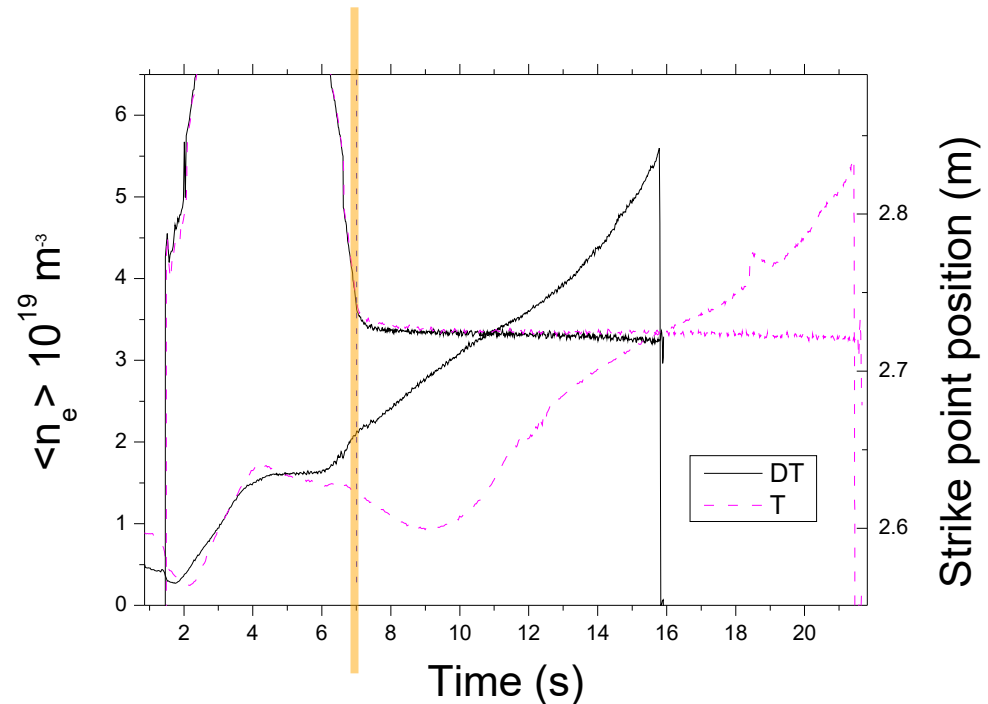# D₂ + T₂ spectrum – procedure

- **Mixed isotopes**

  Brezinsek et al, Physica Scripta.
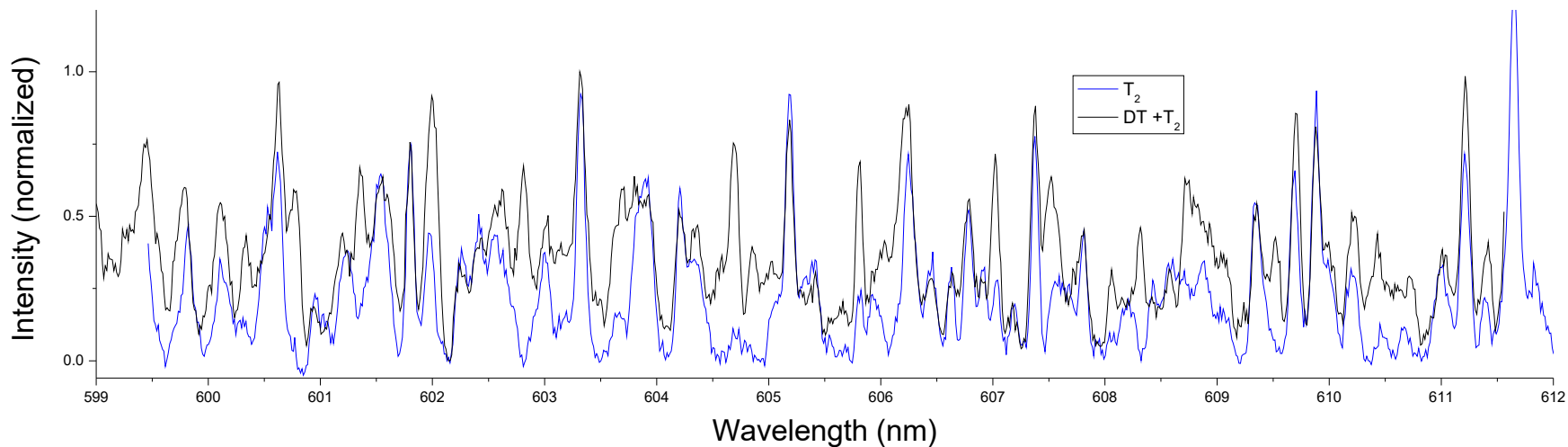 *Vol. T103, 63–67, 2003*

- **So in 60:40 T₂:D₂ mixture – over 50% T₂, 30% DT, below 20% D₂ – D virtually invisible, T dominant, DT visible**
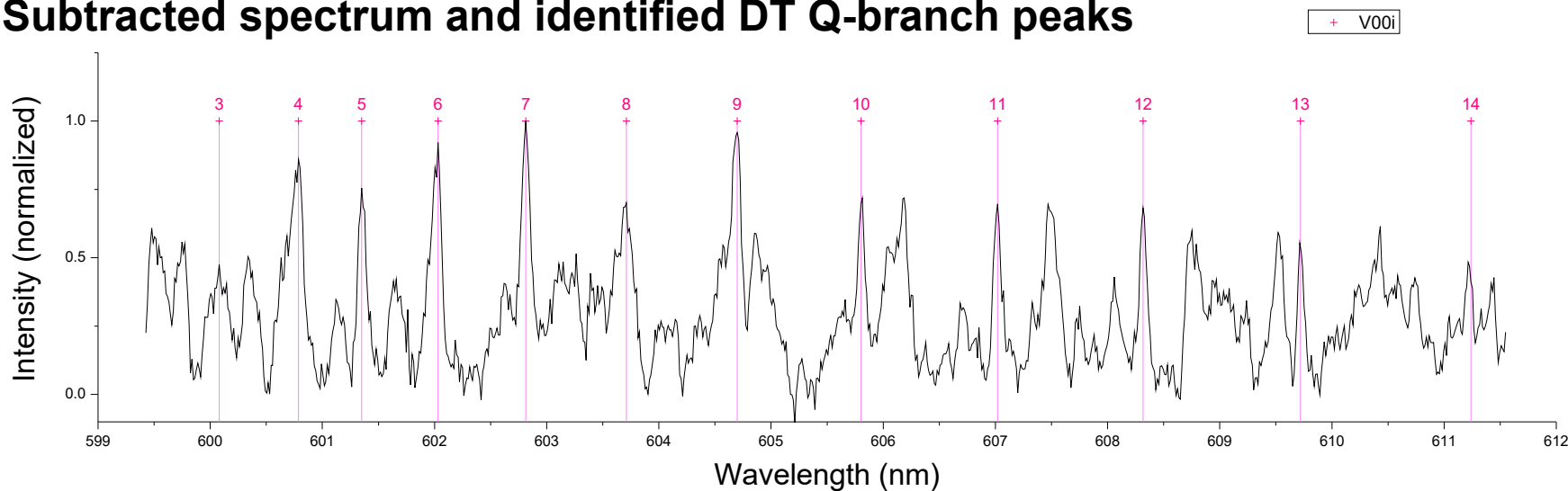
- **7 s into the pulse – comparable conditions**

DT molecule – Q branch peaks

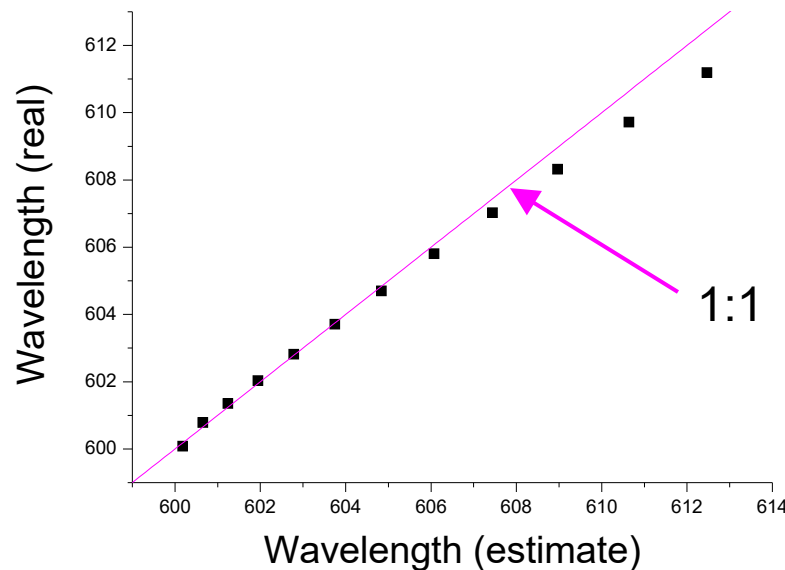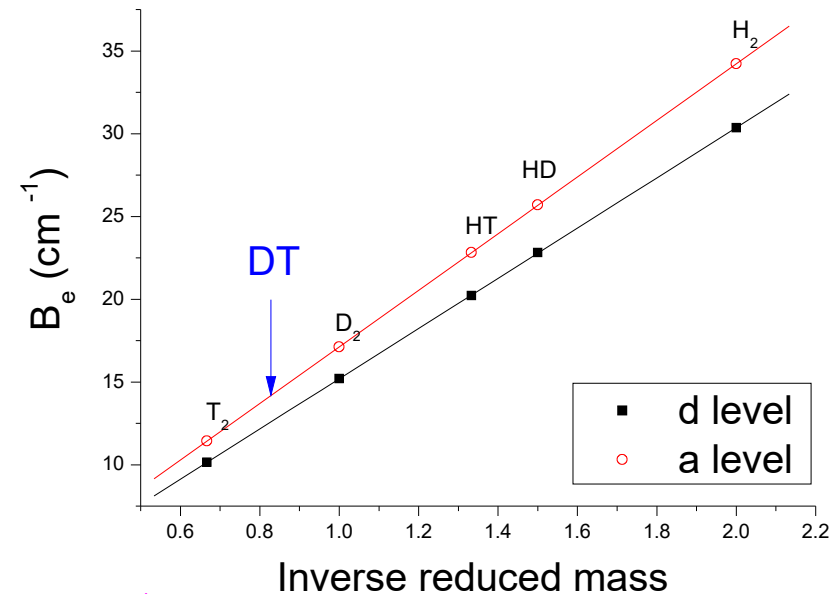**#99433 at 7s: no visible deuterium peaks, only T_2 and DT**

Subtracted spectrum and identified DT Q-branch peaks
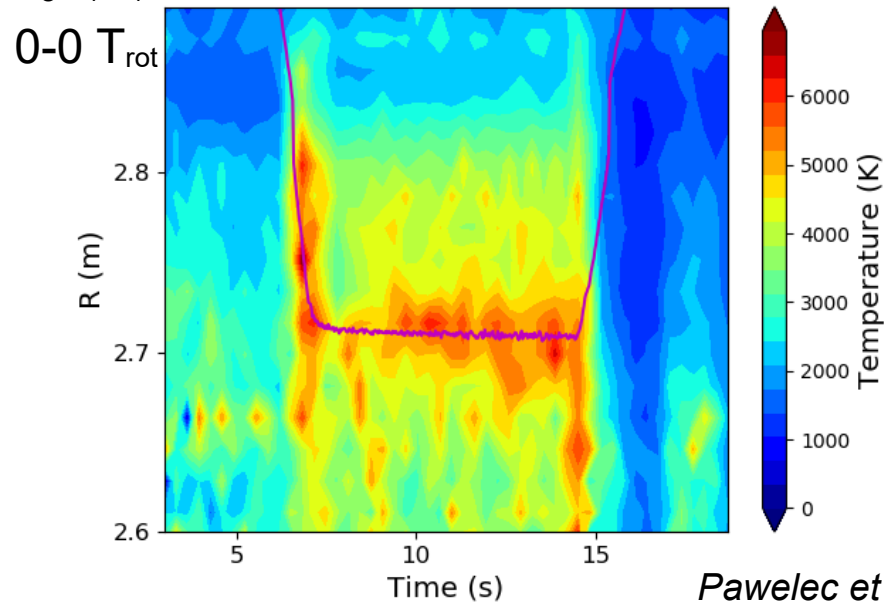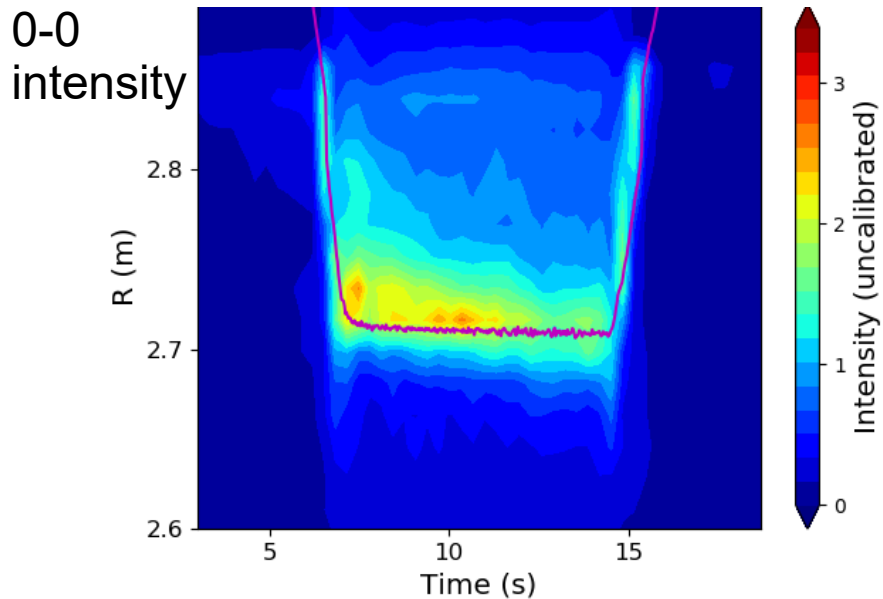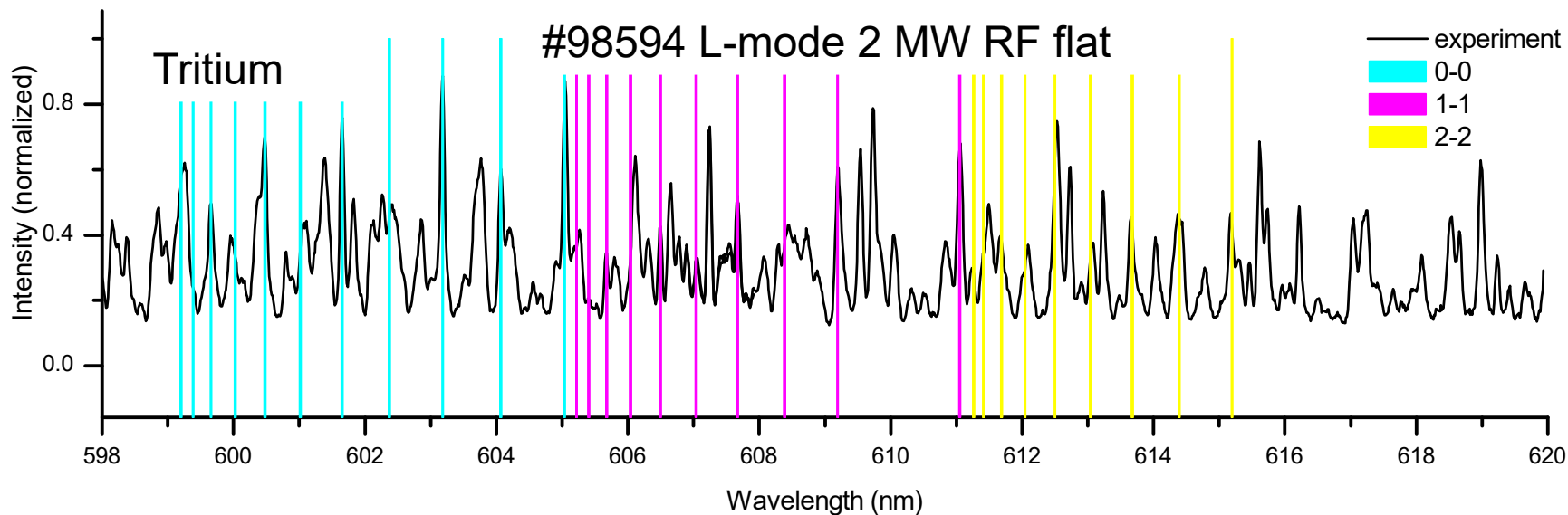
Isotope effect and identification

- Estimation of DT parameters – scaling by inverse reduced mass (for B_e, D_e)

- Estimation and reality difference – D_e value (does not scale completely linearly)

Huber and Herzberg, in NIST Chemistry webbook https://doi.org/10.18434/T4D303,

T₂ analysis

#98594 L-mode 2 MW RF flat

Tritium

experiment — 0-0 (cyan), 1-1 (magenta), 2-2 (yellow)
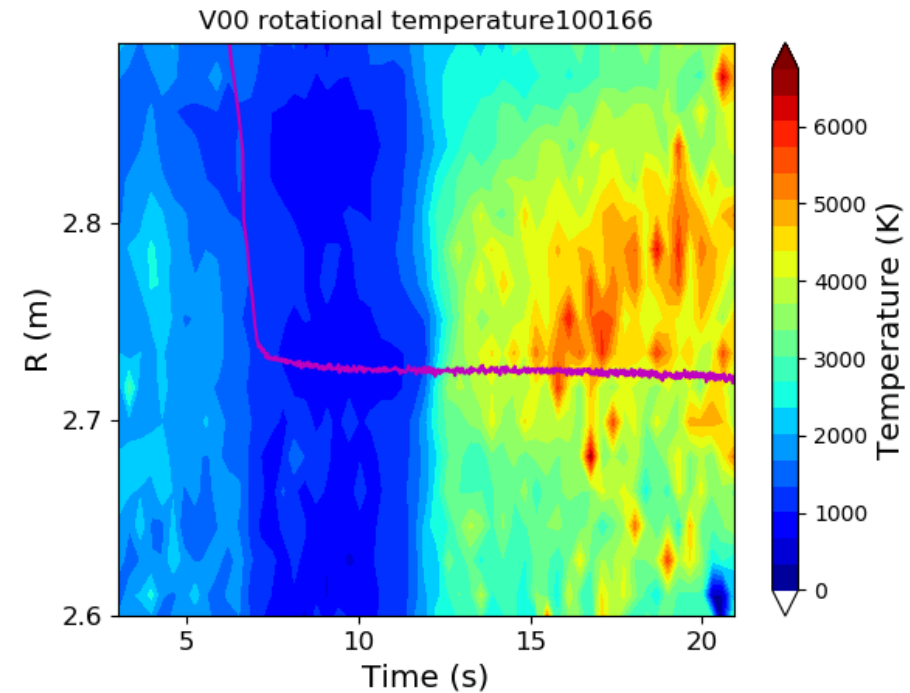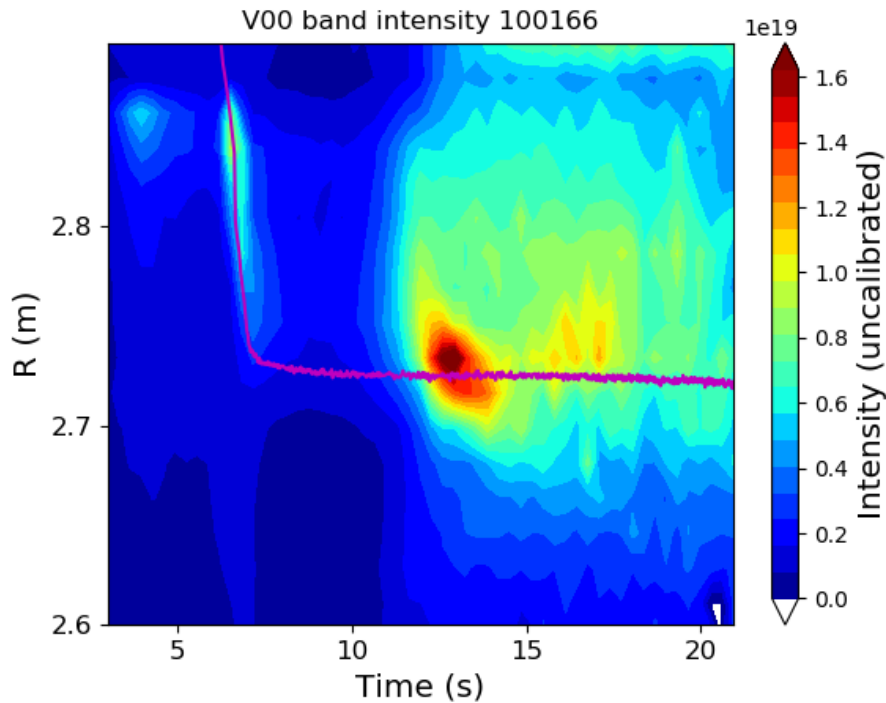
0-0 intensity

0-0 T_rot

Pawelec et al, EPS 2022

T₂ analysis for a density scan #100166

**Boltzmann plot with lines Q(3,5,7,9,11,13)**

One more line used than for #98594, results also up to 5000 K,
but for low density even down to 1000 K!

Profiles

- For 8-10 s very low temperature – even below 1000 K, flat intensity distribution

- For 12-14 s – sharply increasing rotational temperature (reaching 3-4 K), intensity centered on the strike point and just outside it

- For >14 s – temperature stabilization, intensity decrease
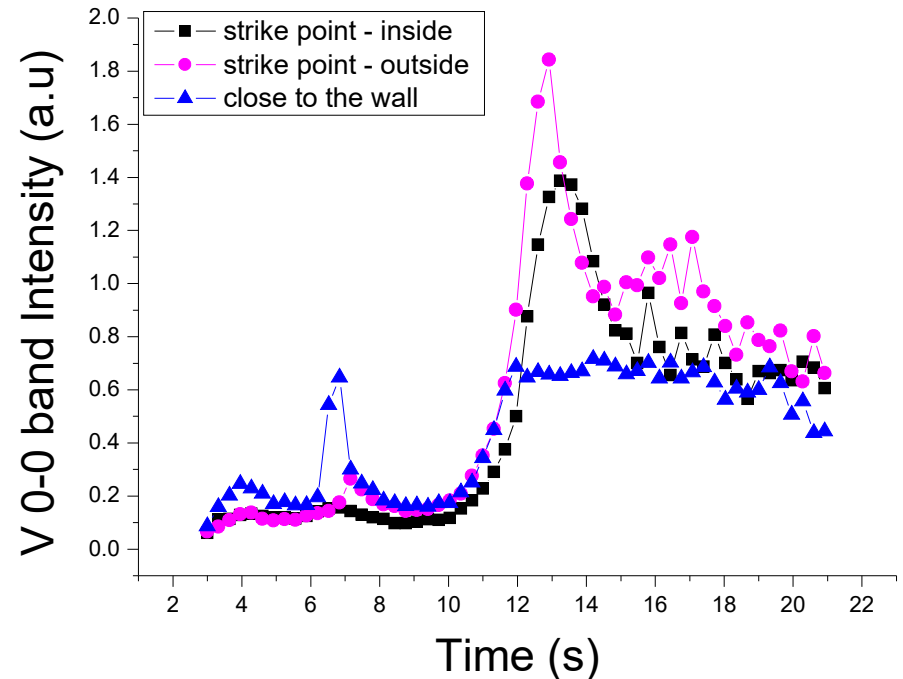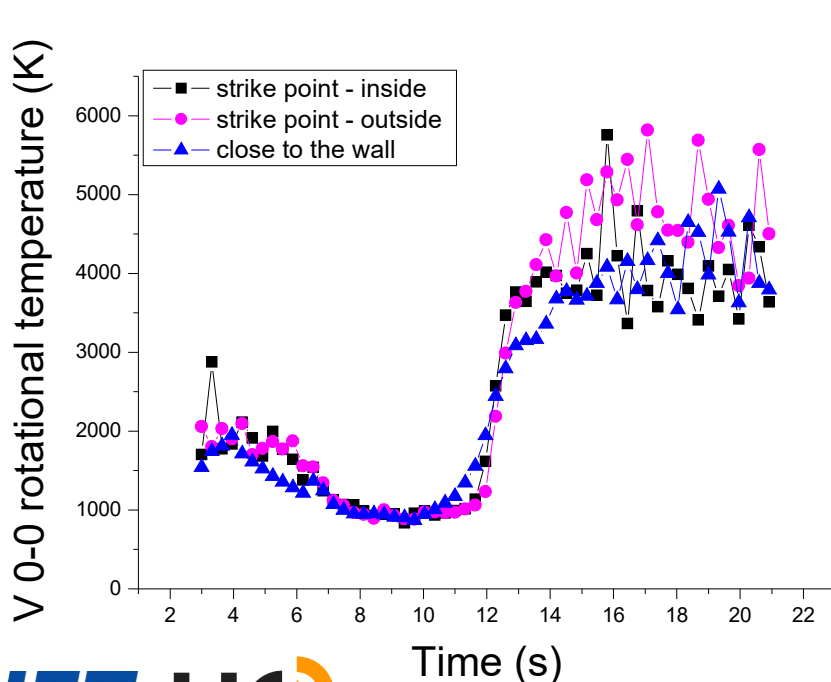
Density correlation

- ## Rotational temperature:

  - Low density – different during density decrease and increase

  - Attached conditions – increase with density

  - For strike point – flat 1000 K for 1-2 10^{19} m^{-3}

  - Detached conditions – large scatter, bulk radiation?

- ## I_{00} intensity

  - Relatively flat for low density

  - Centered on strike point for intermediate density/attached

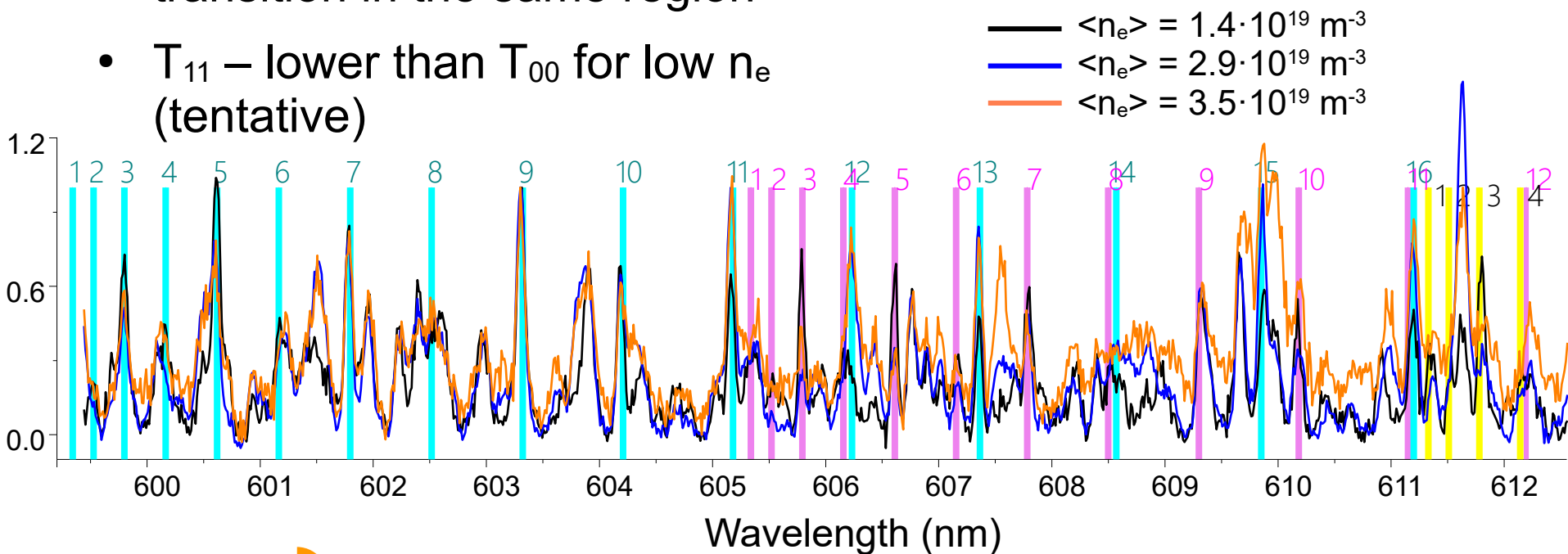 - Spreads out and descends during detached conditions
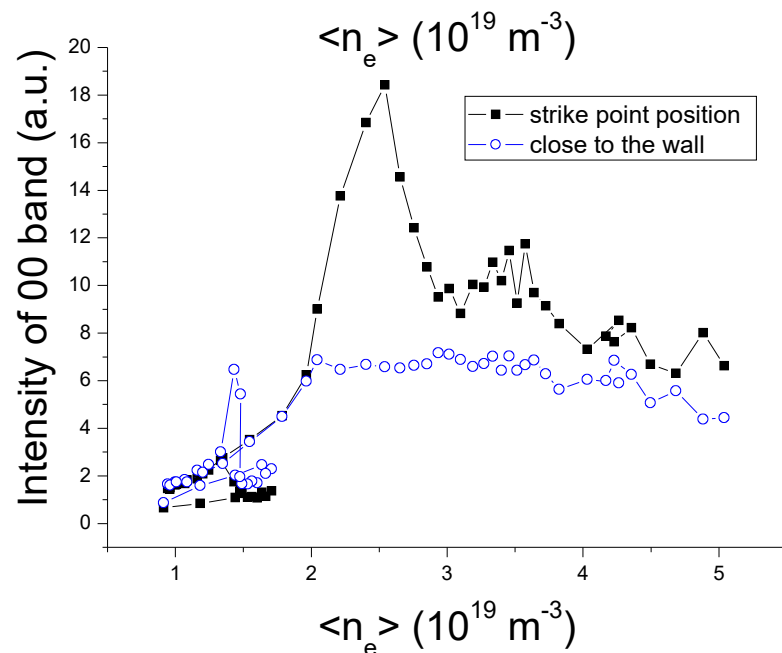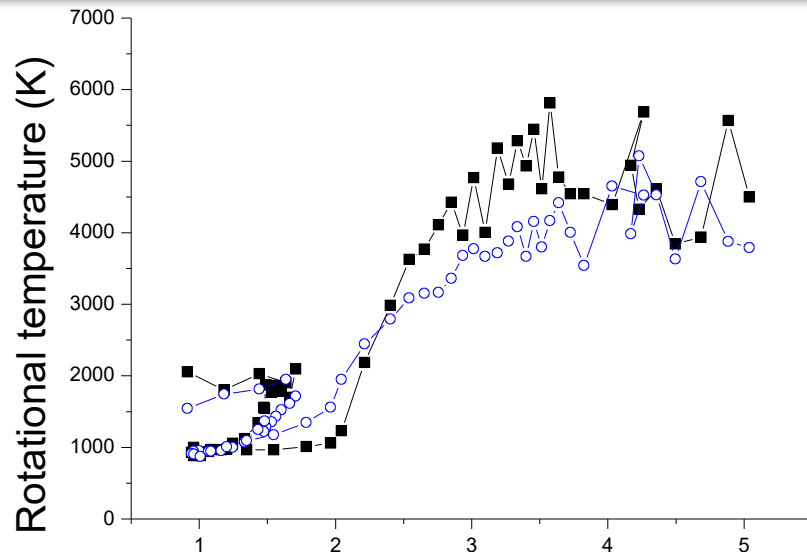
Attached region – ion flux correlations
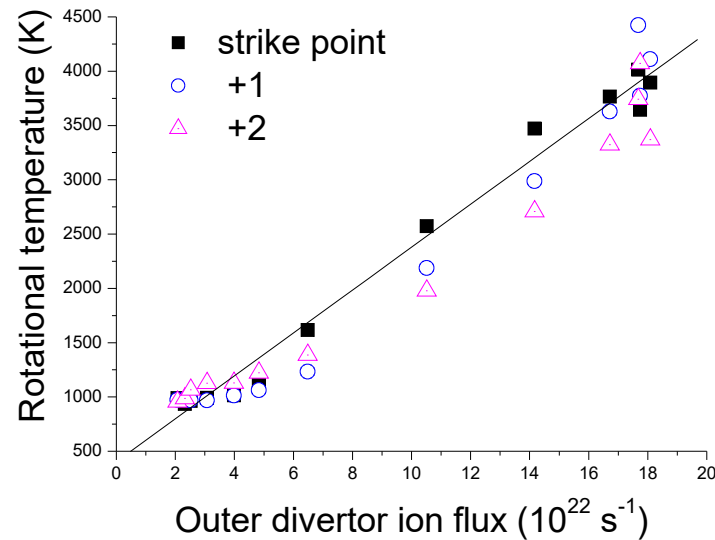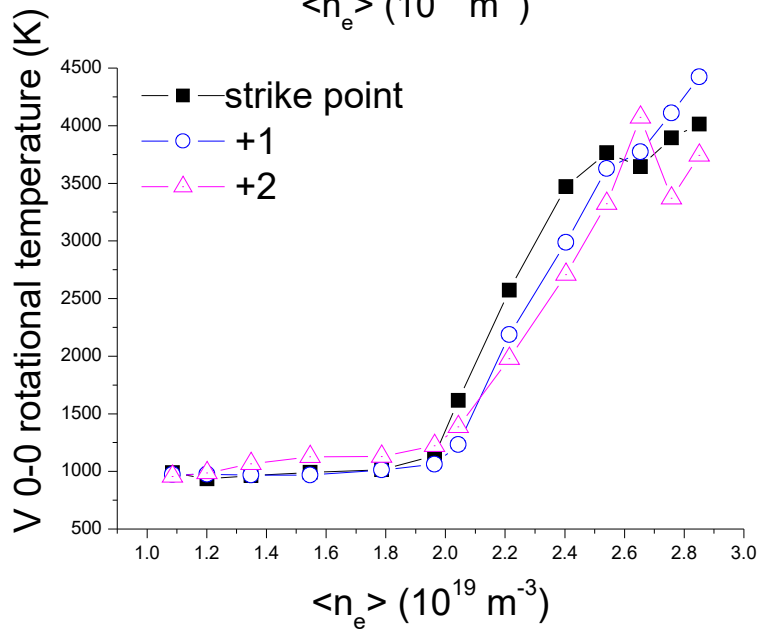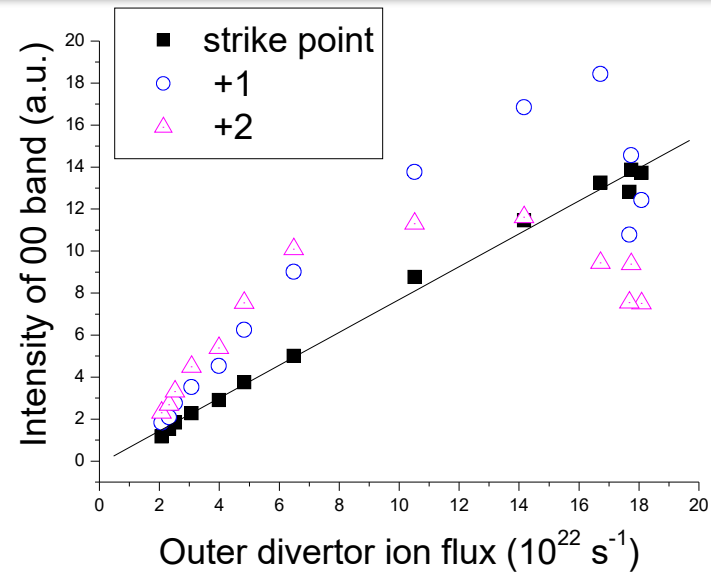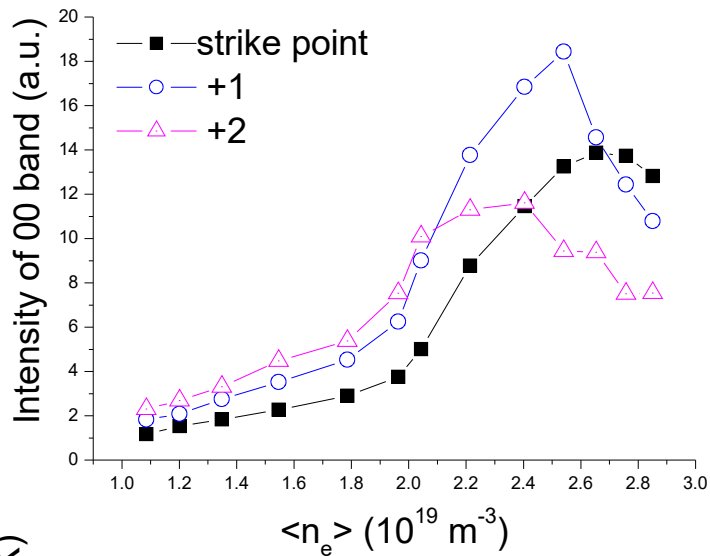
Main challenges

- Very rich spectra, only 6 rotational lines of V 0-0 transition can be considered for Boltzmann plot – large error bars especially for high temperature

- Transitions from higher levels – even less, 1-1 two/three

- Admixtures probably from different molecular levels – g to c transition in the same region

- T_{11} – lower than T_{00} for low n_e (tentative)

Legend:
- $\langle n_e \rangle = 1.4 \cdot 10^{19}$ m^{-3} (black)
- $\langle n_e \rangle = 2.9 \cdot 10^{19}$ m^{-3} (blue)
- $\langle n_e \rangle = 3.5 \cdot 10^{19}$ m^{-3} (orange)
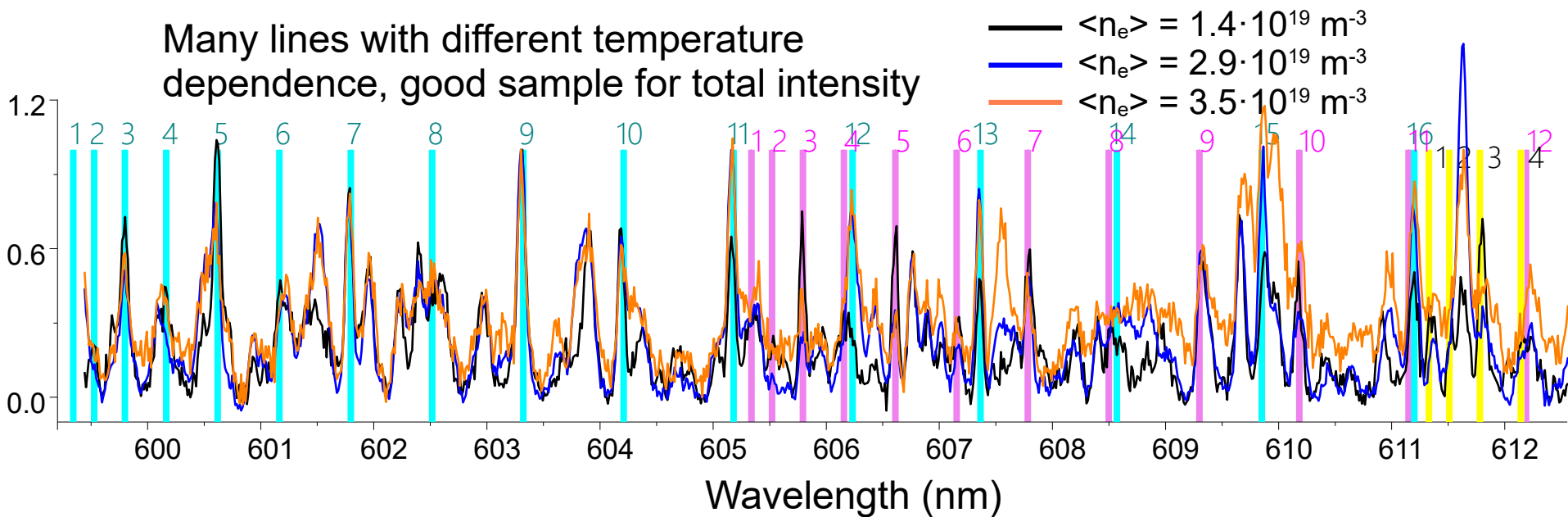
Wavelength (nm)

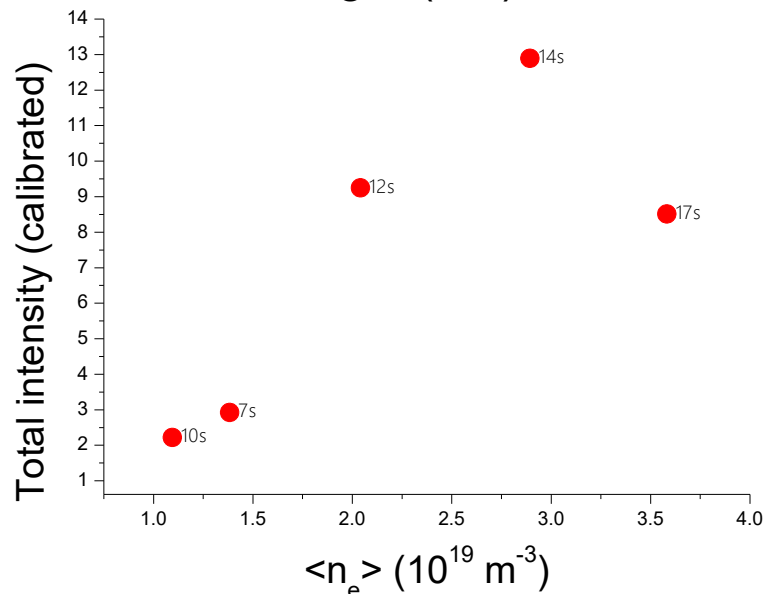# Total band intensity estimation and results

Integrated intensity for tritium

Many lines with different temperature dependence, good sample for total intensity
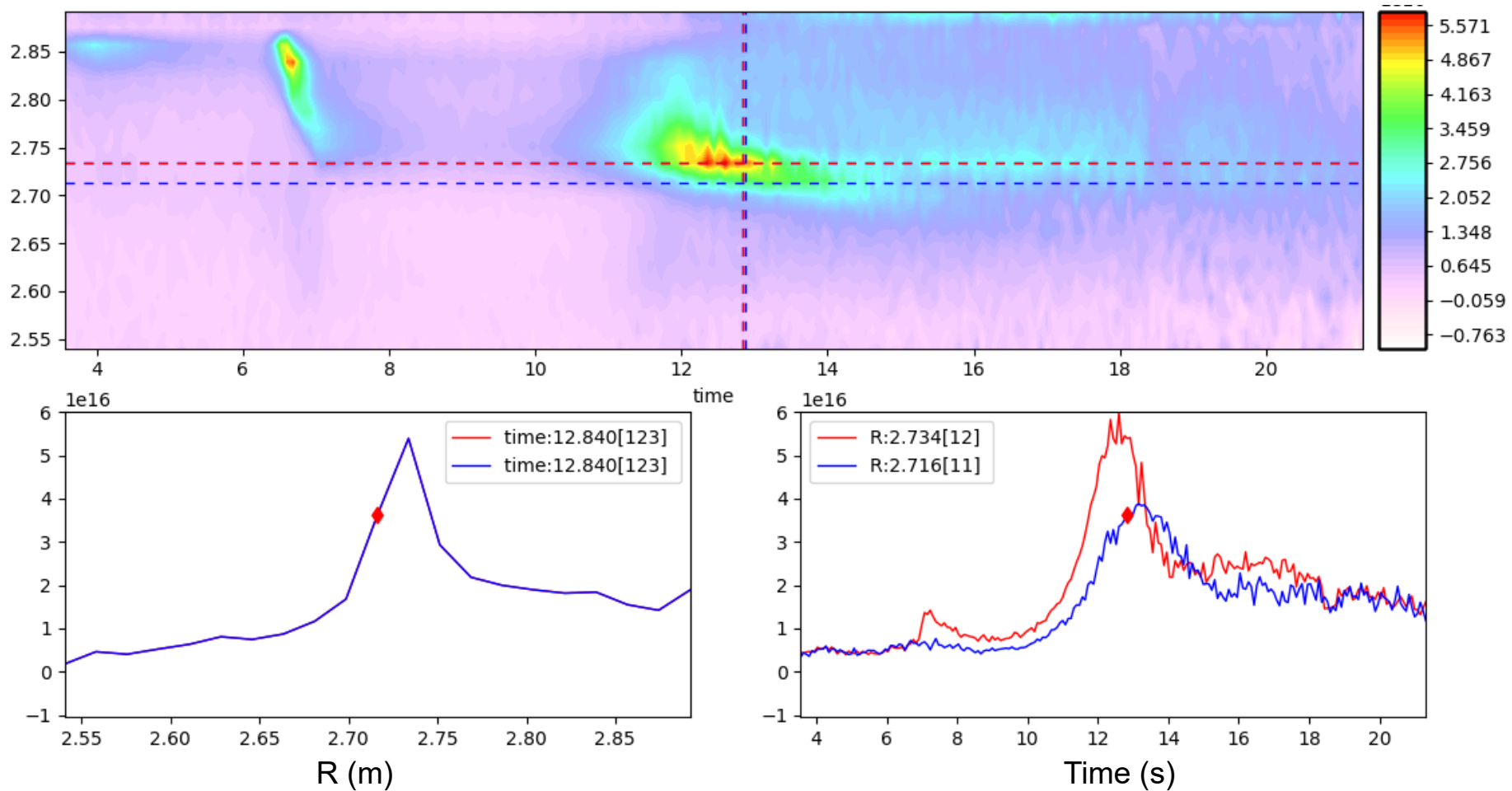
Scale of total intensity for different averaged edge density:
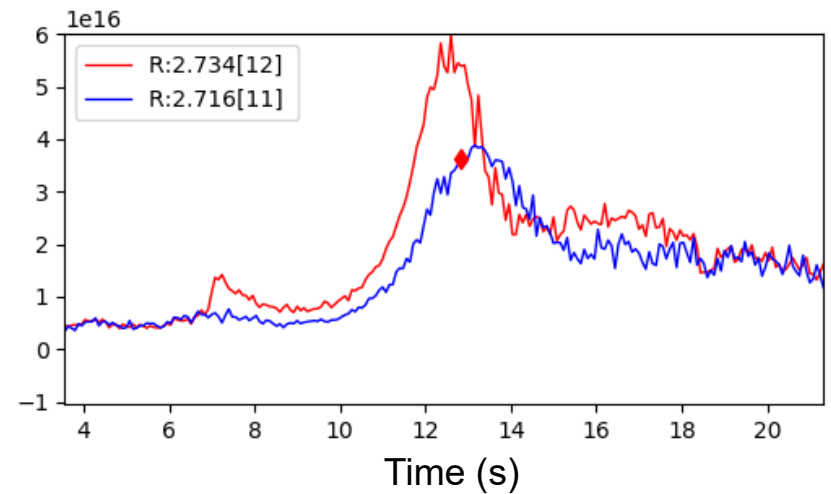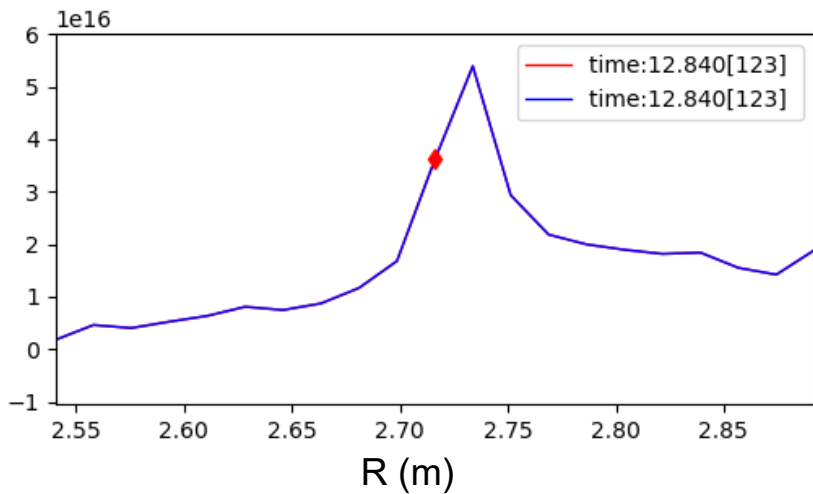
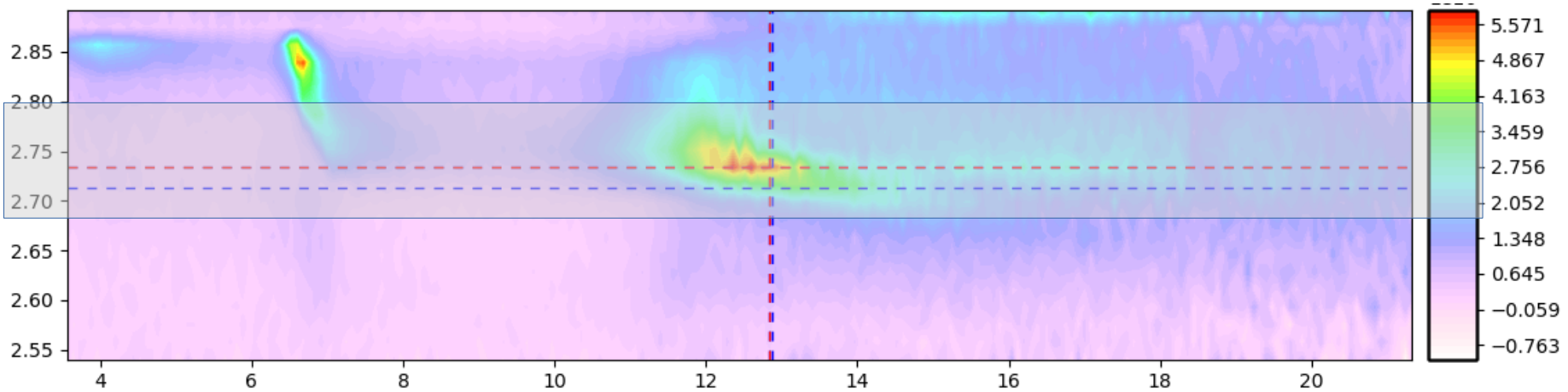# Spatial and temporal distribution

Blue/red – two sides of strike point position

Spatial and temporal distribution

Blue/red – two sides of strike point position

Connection to outer divertor ion flux

- Total T_2 band intensity increases and decreases with ion flux to the surface, but the maximum is not in the same time (time, balance of excitation, electron temperature?)

- Pre-detachment – strong correlation between flux and FB intensity, detached conditions – also correlation, weaker
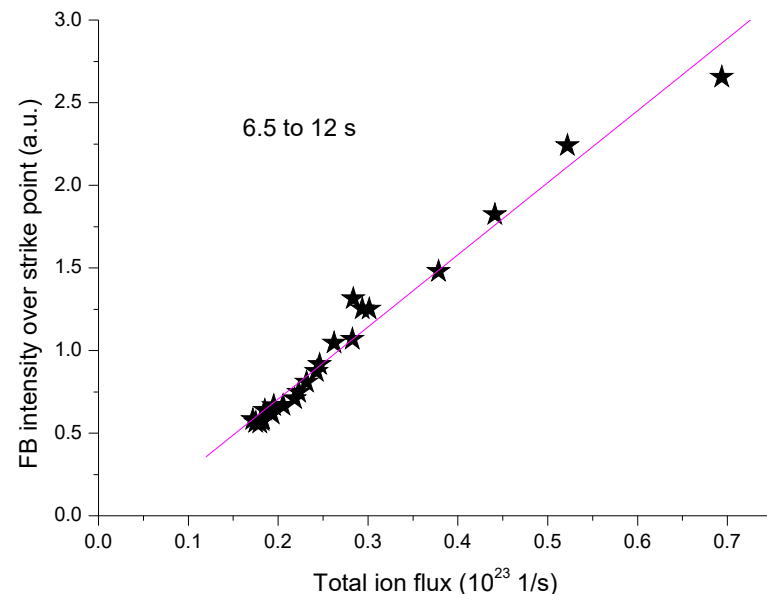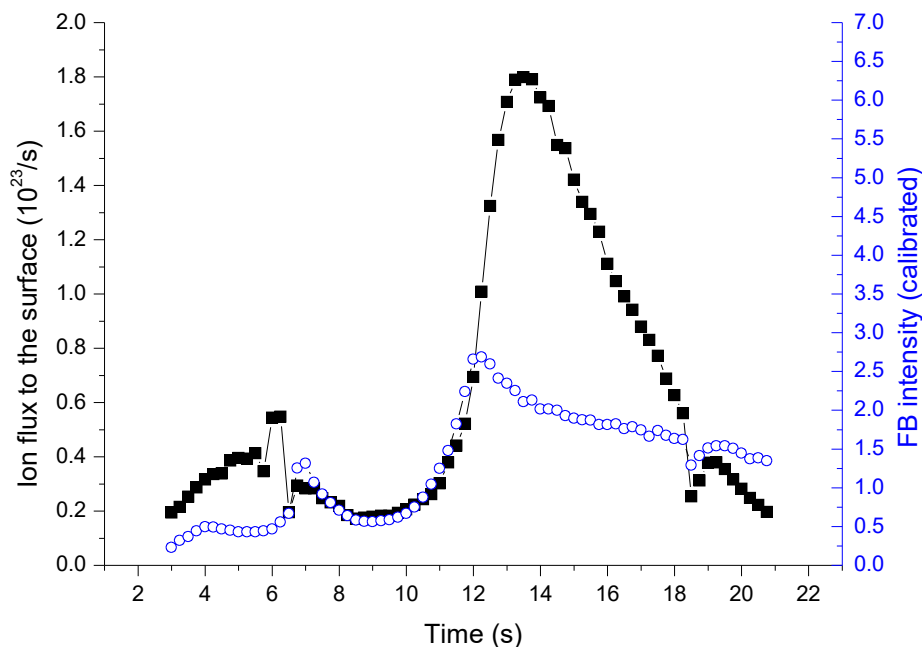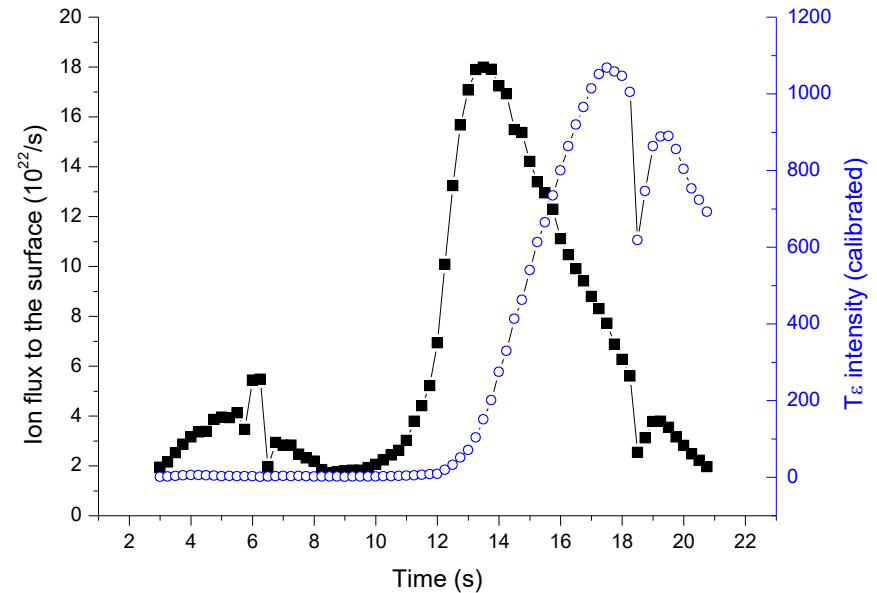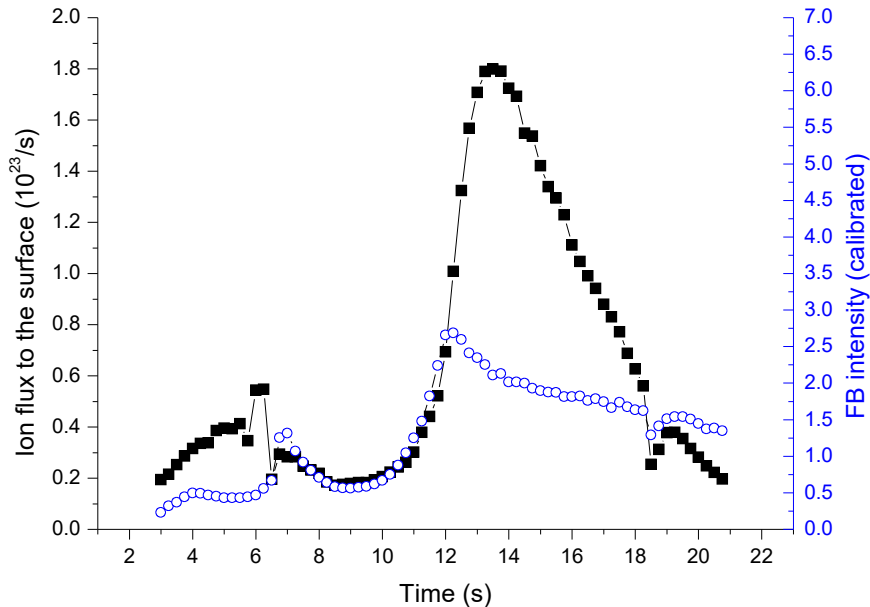
Two branches – low and high rotational temperature /high and low T_e (from over 50 eV, to 6 eV)
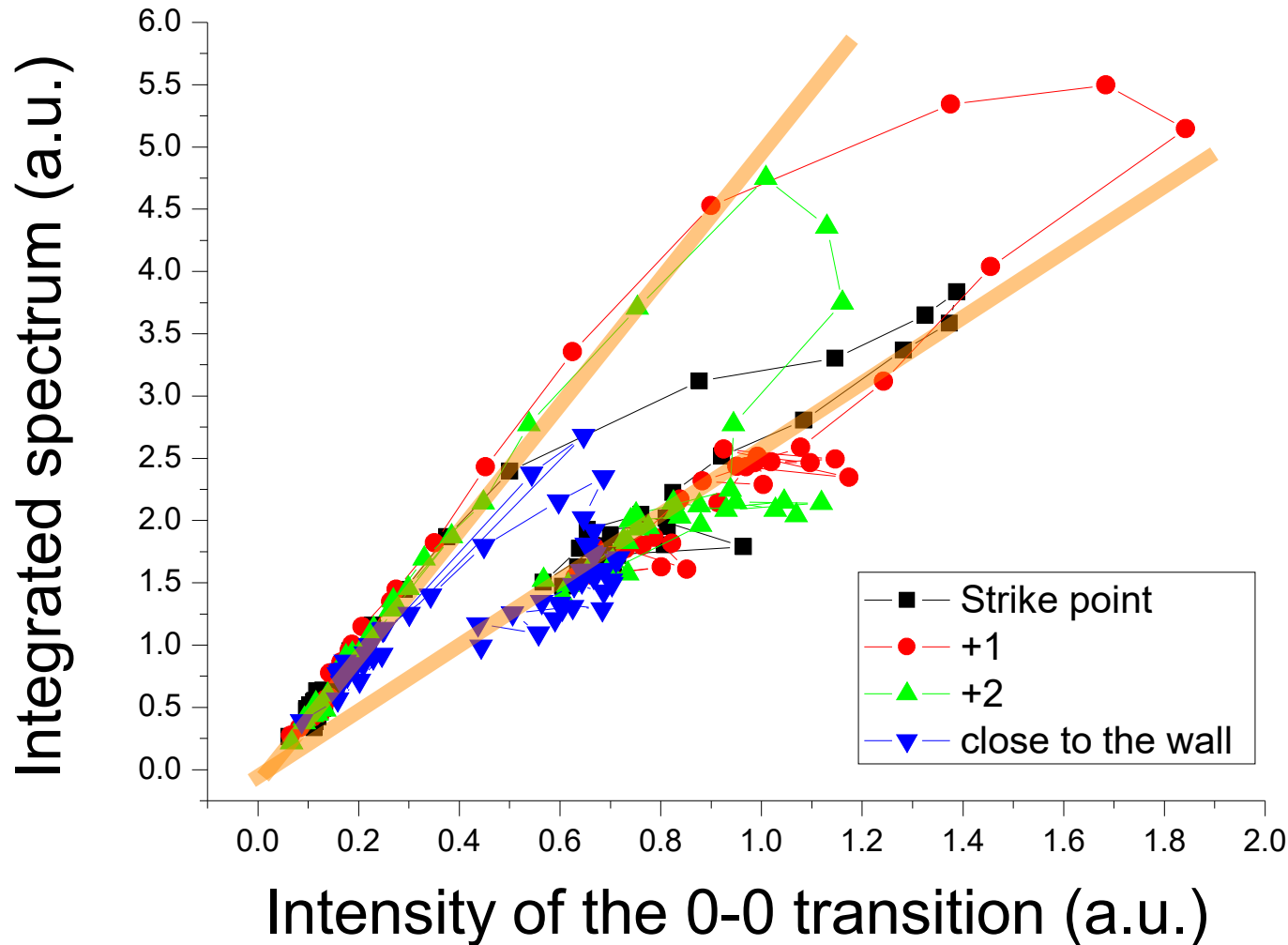
FB bands and atomic lines

- Fulcher band pretty well correlates with ion flux, T_ε line much more connected with density

Summary

- Analysis of the detailed spectra:

  - DT molecular spectrum – measured and Q (0-0) peaks up to 14 identified

  - T_2 too dense for using the Q lines for a clear Boltzmann plot, for any transitions outside 0-0 and even for that the error bar for higher temperature is large

  - Still, density scan shows strong dependence of T_{rot} on density and total ion flux to the surface, especially for attached conditions

- Analysis of the integrated spectrum:

  - Integrated FB spectrum of T_2 within one wavelength range of the available spectrometer can be used for estimating the spatial and temporal dependence of the band behaviour during a density scan

  - There are correlations between integrated and I (0-0) spectrum

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