

Precision in ADAS – some issues arising from spectral fitting using GCR data

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Motivation and background

We have generally considered ADAS to be a reaction database.

- Collection of data for modelling transport and diagnosing emission.
- We 'know' which element and which transitions are under study.
- adf11 PLT, adf15 PECs, adf12 CX emissivities, or Zeeman features are catalogued and compared to *identified* energy-integrated or spectroscopic measurements.
- High precision wavelengths are not required for population modelling.
- Spectral synthesis was not a priority for ADAS.
- Effort was directed to improving *y*-axis accuracy.

Reasons to question/re-assess this stance:

- The experimental measurements we want to confront are complex features.
- Remove a degree of freedom in fitting models of spectral lines.
- Variations in the underlying structure are now noticeable in the derived emissivity and power coefficients.
- Part of concerted approach to quantifying uncertainty.

Note that this does not mean that ADAS will try to replace/compete with NIST (ASD).





Charge exchange BeIV (6-5) multiplet



- Doppler shift of CX feature is a measure of the plasma rotation.
- What is the measurement limit due to precision of the wavelengths of the component lines?
- The energy levels of one-electron ions are known to 0.02cm⁻¹ and are considered better than any spectroscopic measurement.
- 0.06Å shift ~ 3km/s.
- Precision in lambda important for rotation but not CX derived quantities.

Method	Wavelength (Å)
Erickson statistical weighted	4658.68537
Uncertainty in Erickson	0.00011
ADAS statistical weighted	4658.68555
ADAS emission weighted	4658.62598
Centroid of ADAS Doppler feature	4658.623

Satellite lines



Rice et al, J. Phys. B, 44 (2011) 165702

- Doppler shift of CX feature is a measure of the plasma rotation.
- What is the measurement limit due to precision of the wavelengths of the component lines?
- The energy levels of one-electron ions are known to 0.02cm⁻¹ and are considered better than any spectroscopic measurement.
- Distortion of Ly-α must be accounted for in fitting at < 10% level.
- High precision in wavelength of satellites and high quality DR rate for intensity is essential.



Types of Tungsten spectra



- Ni-like, 3d¹⁰ ground state, one active electron Nakano et al, J Phys. B, 144023 (2015).
- W³⁴⁺ to W⁴⁵⁺ in JET soft X-ray.
- W (Z=74) and Hf (Z=72) in JET VUV
- Wavelength precision important for analysing features.
- Theoretical or EBIT measured λ-basis set.
- Excitation calculations for intensity.



Spectral synthesis



- ADAS does have the tools for spectral synthesis Atomic Data and Analysis Structure
- PECs for line intensity, fortran/IDL routines for λ -resolved continuum.
- Sufficient for diagnostic design but better wavelength precision for fitting.



Fitting a solar Fe²⁺ multiplet



3d⁶ ³H – 3d⁵(4G)4p ³H

E	dlén	R-matrix (optimized)
 3H_6 200 3H 5 203		23018.5179 23235.0067
3H_4 204	481.1	23451.3811
and		
3H_6 118	354.21	127294.3864
3H_5 118	556.45	127673.1821
3H_4 118	685.45	127878.7733

- R-matrix collision data: Badnell, Ap. J, 785, 99, (2014)
- NIST energy levels: Edlén, Ap. J, 95, 532, (1942)
- Match energy levels with adas7#5
 - adf04/nist#26/ic#fe2.dat and adf04/crlike/crlike_nrb13#fe2.dat
- Fit with ADAS ffs/afg framework.

Conclusions

- Precision in intensity has been the focus of ADAS.
- Precision in wavelength has not been a priority or a necessity.
- In some cases mostly involving spectral features high precision in wavelength is now required.
- Improvement is a pre-processing step of the analysis.
- Develop ADAS tools to assist
 - collection of spectroscopically accurate adf04 data (from NIST)
 - software routine to match these to adf04 data
 - and to fill-in for sparse primary NIST data

