DOUBLY-IONISED IRON (Fe III): New Accurate Wavelengths and Energy Levels

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See this poster online here:

"Multimillion-dollar projects… are producing data that cannot be analysed because of a failure to support much cheaper lab work on the ground." Nature Editorial, 503 437 (2013)

We take requests for atomic data!

Atomic Data Needs in Astronomy

Accurate atomic data is essential for the successful analysis of modern astronomical spectra. However, some of the astrophysically important elements have incomplete or inaccurate atomic data, which can result in the misidentification of spectral lines, incorrectly calculated elemental abundances, or the inability to dis-entangle blended lines.

Details of the **Laboratory Astrophysics Programme at Imperial College London** can be found at Concepcion et al., 2023.

The Spectroscopy group at Imperial College are focusing on **iron-group** elements (and **neodymium**, see Milan Ding's poster) as many are in urgent need of atomic data revision and improvement. Their **high cosmic relative abundances** and **complex atomic structure** result in the production of many spectral lines between the **vacuum-ultraviolet** (VUV, <200 nm) and **infrared** (IR), and account for the majority of opacity in stars.

The wavelengths we measure are used in the creation of linelists for many spectroscopic surveys, including the Gaia-ESO Spectroscopic Survey for the study of Galactic Evolution (Gilmore et al., 2022, Randich et al., 2022). Our Co I HFS (Pickering, 1996) and Fe I transition probabilities data (Ruffoni et al., 2014) are included in the Gaia-ESO line list (Heiter et al., 2021).

New instrument!

The IC Spectroscopy group have recently purchased a Bruker IFS 125HR spectrometer optimized for measurements from the visible to mid-IR spectral regions, from 1850-25,000 cm^{-1} (400nm to 5.4 μm). This spectrometer will complement the IC VUV FTS, allowing us the **capability to measure FT spectra from the VUV to the mid-IR**. Delivery is due mid-2023.

High-resolution Fourier Transform Spectroscopy

At Imperial College (IC), we use the vacuum-ultraviolet (VUV) Fourier transform (FT) spectrometer to investigate atomic spectra. The instrument has

- **Spectral range: 140 - 840 nm**
- **Resolving power: ~2 million at 200 nm**

Beyond the this spectral range, we supplement our measurements with data recorded at **NIST** (USA).

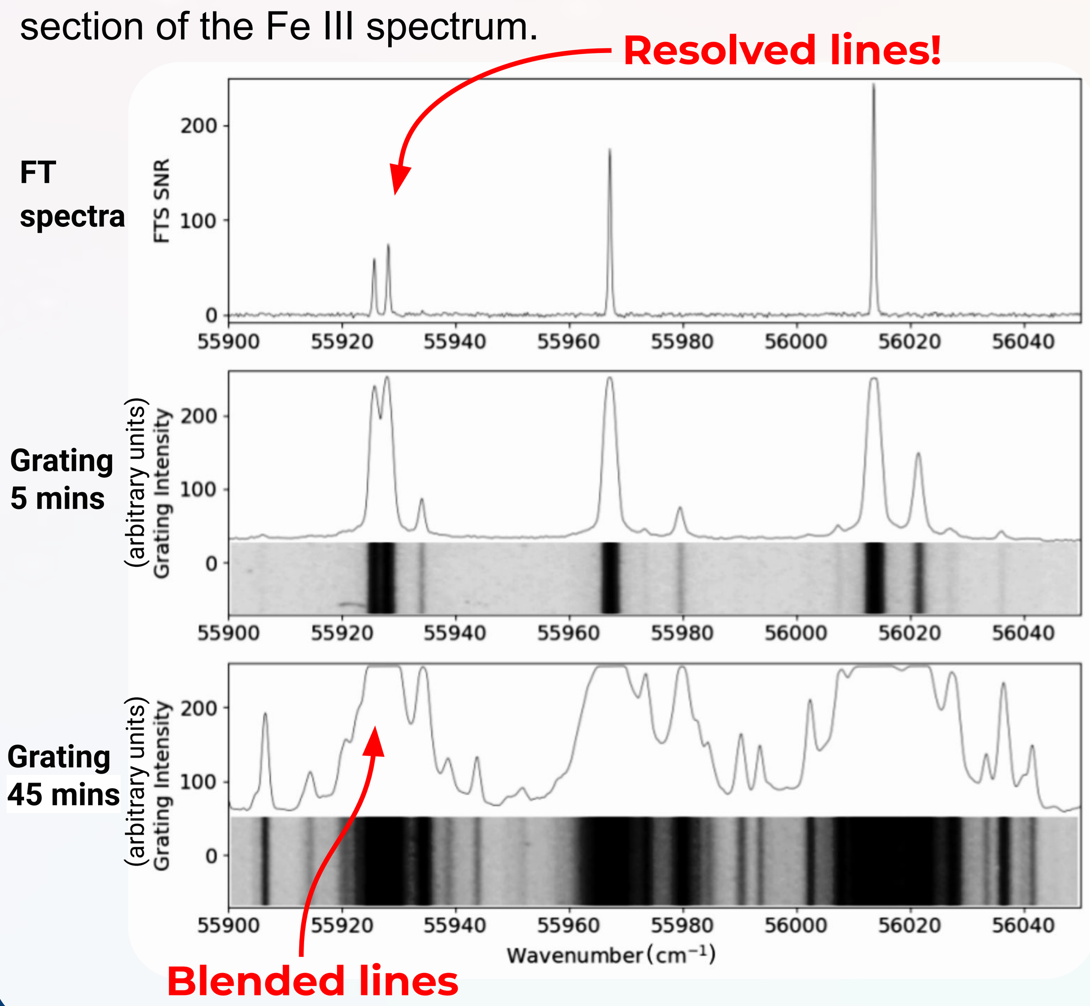
FT spectra provides accurate transition wavelengths, which are used to improve known level energies and search for unknown levels. We measure:

- **Wavelengths** and **energy levels** accurate to at least 1 part in 10^7 (30 ms^{-1}, 0.015 nm at 150nm),
- **log(gf)s** (a.k.a. **transition probabilities** or **oscillator strengths**) accurate to a few percent,
- Data for line broadening effects such as **hyperfine structure** and **isotope structure**, down to the order of a few 10^{-3} cm^{-1}.

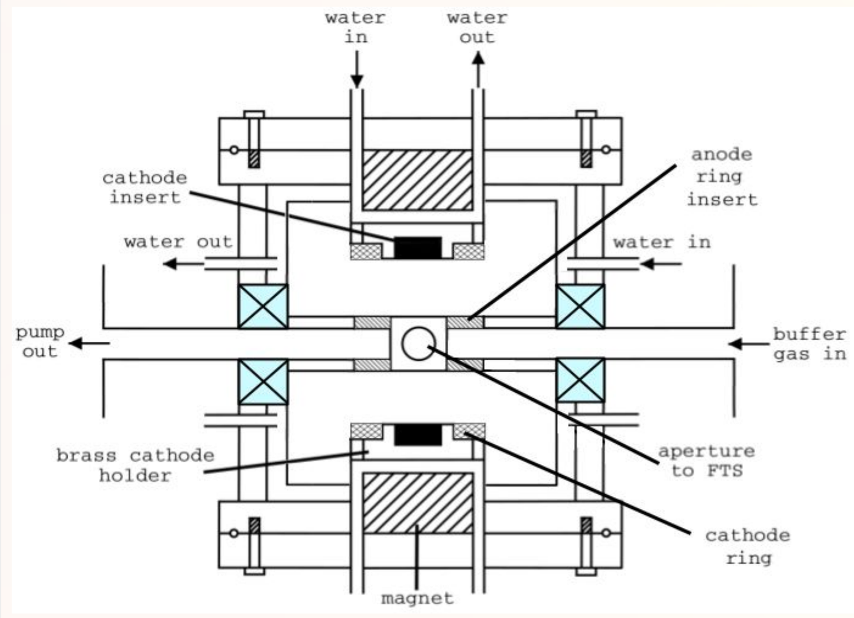
The FT spectrometer is capable of resolving line broadening effects such as hyperfine structure and isotope structure. Please see Milan Ding's poster for more information.

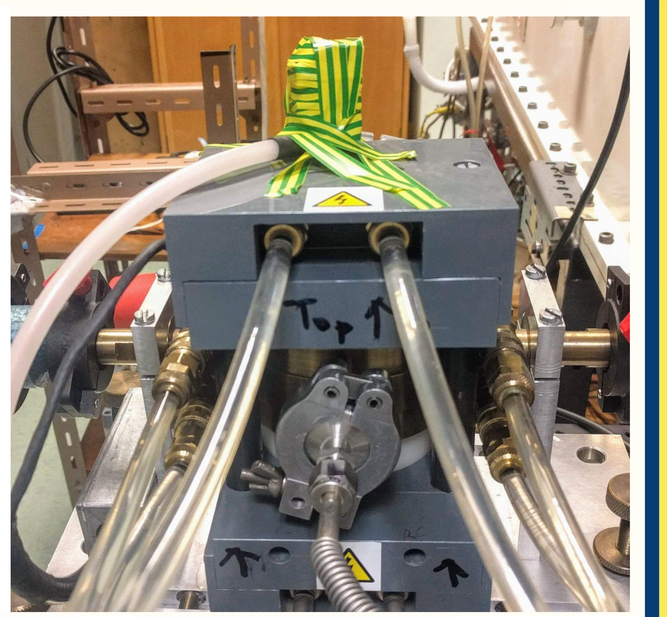
FT vs Grating Spectra

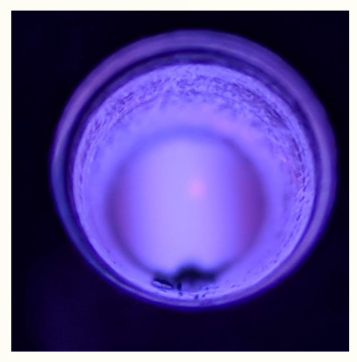
For Fe III, the previously published data were measured using grating data. FT spectroscopy improves the accuracy of wavelengths and energy levels by at least an order of magnitude over the previous results. Below is a comparison of the resolving power between FT and grating data for a section of the Fe III spectrum.

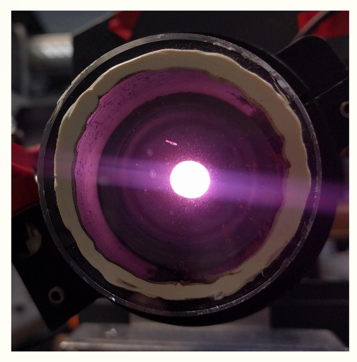


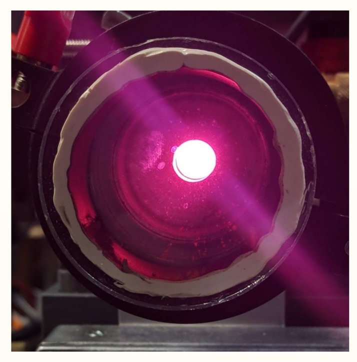
Light Source: Penning Discharge Lamp











FT spectroscopy requires stable light sources. We use a **Hollow cathode discharge lamp** for neutral and singly-ionised elements and a **Penning discharge lamp** (PDL) for doubly-ionised elements.

Above is shown a schematic diagram (left) and a picture of the PDL (right). In the PDL, a large potential is applied to the cathodes located on either side of the grounded central anode ring. The metal cathodes are sputtered by a steady flow of low pressure gas, emitting electrons which are confined to oscillate between the cathodes due to the strong magnetic field applied parallel to the electric field (creating a Penning trap!). These high energy electrons ionise the buffer gas, leading to the bombardment and excitation of the metal from the cathodes. To the right are pictures of the PDL plasma produced with high purity iron cathodes (99.8+%): [top] close-up picture of plasma with argon; [middle] plasma with neon-helium gas mixture; [bottom] plasma with neon gas.

The recorded spectra are **intensity calibrated** using tungsten and deuterium standard lamps.

Fe III Wavelengths and Energy Levels

Using a PDL, the **first high-resolution FT spectra of Fe III** has been recorded in the UV-VUV region, (153 nm to 296 nm, 33,826 cm^{-1} to 65,508 cm^{-1}), with uncertainties of strong lines (SNR > 50) between 0.0024 cm^{-1} and 0.0074 cm^{-1}. FTS line wavenumbers were calibrated to an accuracy of 5 − 8.5 parts per 10^8 using accurate Fe II Ritz wavelengths produced by Nave & Johansson (2013). This data recorded the wavelengths of transitions between most of the lower-lying 4s and 4p energy levels.

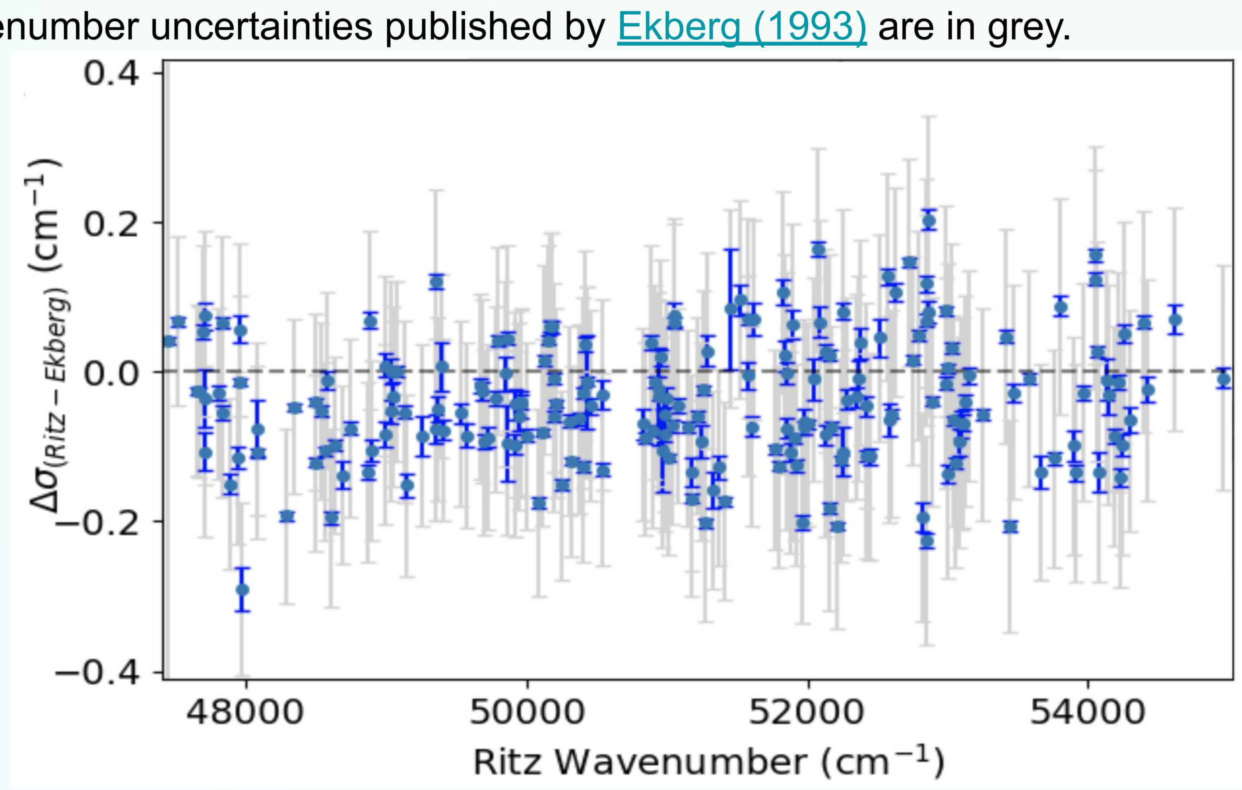
However, in order to connect the system to the lowest-lying $3d^6$ energy levels, transitions further in the VUV region were required. Grating spectral data at high wavenumbers (55,090 cm^{-1} to 163,164 cm^{-1}, 61 nm to 1815 nm) was recorded at the normal incidence vacuum spectrograph (NIVS) at the National Institute of Standards and Technology (NIST) in Maryland, USA.

Using FT and grating spectra, 1890 transitions have been identified as Fe III and 313 Fe III energy levels (3d6, 4s, 4p levels) have been revised and optimised. The Ritz wavenumbers are at least **an order of magnitude more accurate** than previously published values from Ekberg (1993) with 456 wavelengths identified to be of sufficient accuracy to be used as **wavelength standards**. These can be used for the calibration of VUV spectra of hot stars.

Useful for the study of low-density astrophysical plasmas, 432 parity-forbidden Ritz wavelengths have also been re-calculated.

FT spectrometer wavenumbers vs previous data

Below is a comparison of the FT spectrometer measured wavelengths with the previously published Fe III wavelengths by Ekberg (1993) using grating spectroscopy. The FTS line wavenumber uncertainties are in blue and the grating wavenumber uncertainties published by Ekberg (1993) are in grey.



Iron-group Elements Update

Wavelengths and Energy Levels

There have been recent advancements in the measurements of accurate transition wavelengths, the optimisation of previously-known energy levels and the discovery of new energy levels for **vanadium, manganese, nickel** and **neodymium**:

- **Vanadium**: Four new energy levels of **V I** found and nine previously unidentified lines classified. Paper submitted for publication.
- **Manganese**: Using FT spectra, 1284 **Mn I** transitions have been identified and new energy levels are currently being found. Using FT and grating spectroscopy, the identification of 6019 **Mn II** lines (82-5500nm) and the confirmation or discovery and optimisation of 614 **Mn II** energy levels (Liggins et al., 2021a).
- **Nickel**: Using high-resolution FT spectra, 1424 **Ni II** transitions have been identified and used to confirm and optimise 283 previously reported energy levels, with uncertainties reduced by at least one order of magnitude. **25 new energy** levels were also identified for the first time (Clear et al., 2022). For higher-lying energy levels of Ni II, including the $3d^8$(3F) 5f to $3d^8$(3F) 9s configurations, 1016 lines were identified and 208 previously reported energy levels were confirmed and optimized with reductions in uncertainty by at least an order of magnitude. A **new ionization energy** for Ni II has also been derived. Paper submitted for publication. The study into the energy levels of the doubly-excited system of Ni II is underway.
- **Neodymium**: The IC VUV FT spectrometer recorded Nd III in the region 8695-1613nm using both a HCL and PDL (**for the first time**). In the very dense spectrum, 568 Nd III transitions have been identified, determining **180 atomic energy levels** (a huge increase over the 35 previously identified levels!) with uncertainties of a few parts in 10^8. These results are in preparation for publication.

There are also plans to study **neon** and **cobalt**. The progress of iron-group investigations prior to 2020 is reported in Pickering et al., 2020.

Parity-forbidden Wavelengths

By optimising atomic energy levels, Ritz wavelengths of **parity-forbidden** transitions that cannot be observed in a laboratory setting can be calculated. Recent studies include **Mn II** (1130 parity-forbidden lines between 237 nm and 170 μm, Liggins et al., 2021b) and **Ni II** (126 parity-forbidden transitions with uncertainties by up to two orders-of-magnitude lower than previously published values, Clear et al., 2023).

Transition probabilities

Transition probabilities for **Mn II** and **Ni II** using the branching fraction method are underway. For **Sc II**, transition probabilities for 57 lines were determined and used for new solar abundance determination (Pehlivan Rhodin et al., 2017).

Our website: www.sp.ph.ic.ac.uk/~julietp/FTS/

Contact us to find out more!

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