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New Accurate Atomic Data for Astrophysical Applications

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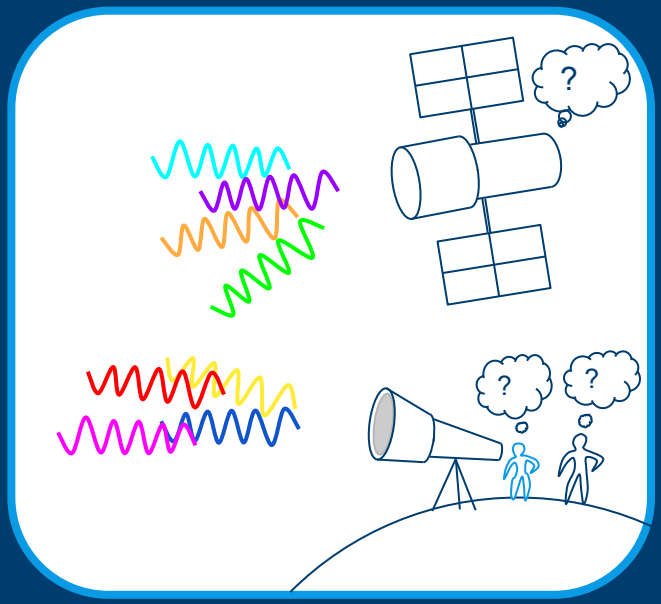
> "Multimillion-dollar projects... are producing **data that cannot be analysed** because of a failure to support much cheaper lab work on the ground."
>
> Nature Editorial [1]

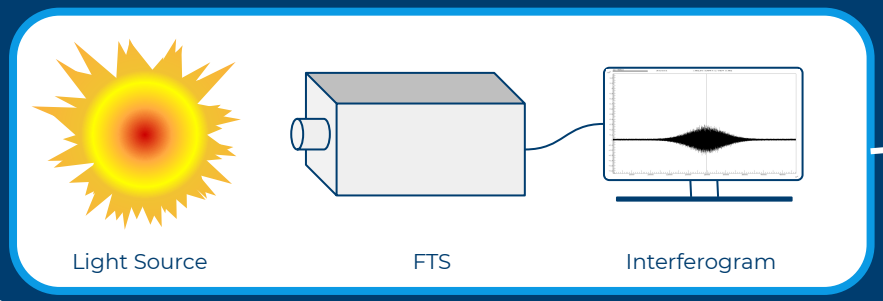


In many cases, the range and spectral resolution of astronomical spectra recorded by ground and space-based spectrographs are now of better quality than available measured atomic data! Accurate atomic data are urgently required.

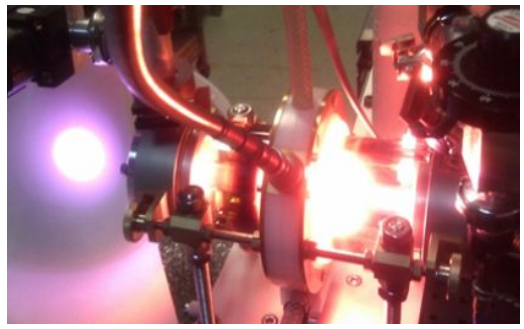
We use the **Fourier Transform Spectrometer** (FTS) at the Imperial College spectroscopy group to measure high resolution spectra.

Spectral range: 140 — 800 nm
Resolving power: ~ 2 million at 200 nm

Beyond this spectral range, we supplement our measurements with infrared (IR) FT spectra recorded at NIST (USA) and Lund University (Sweden), and vacuum ultraviolet (VUV, < 200 nm) Grating spectra recorded at NIST (in collaboration with G. Nave).



Fourier Transform for spectrum



Running Hollow Cathode Lamp

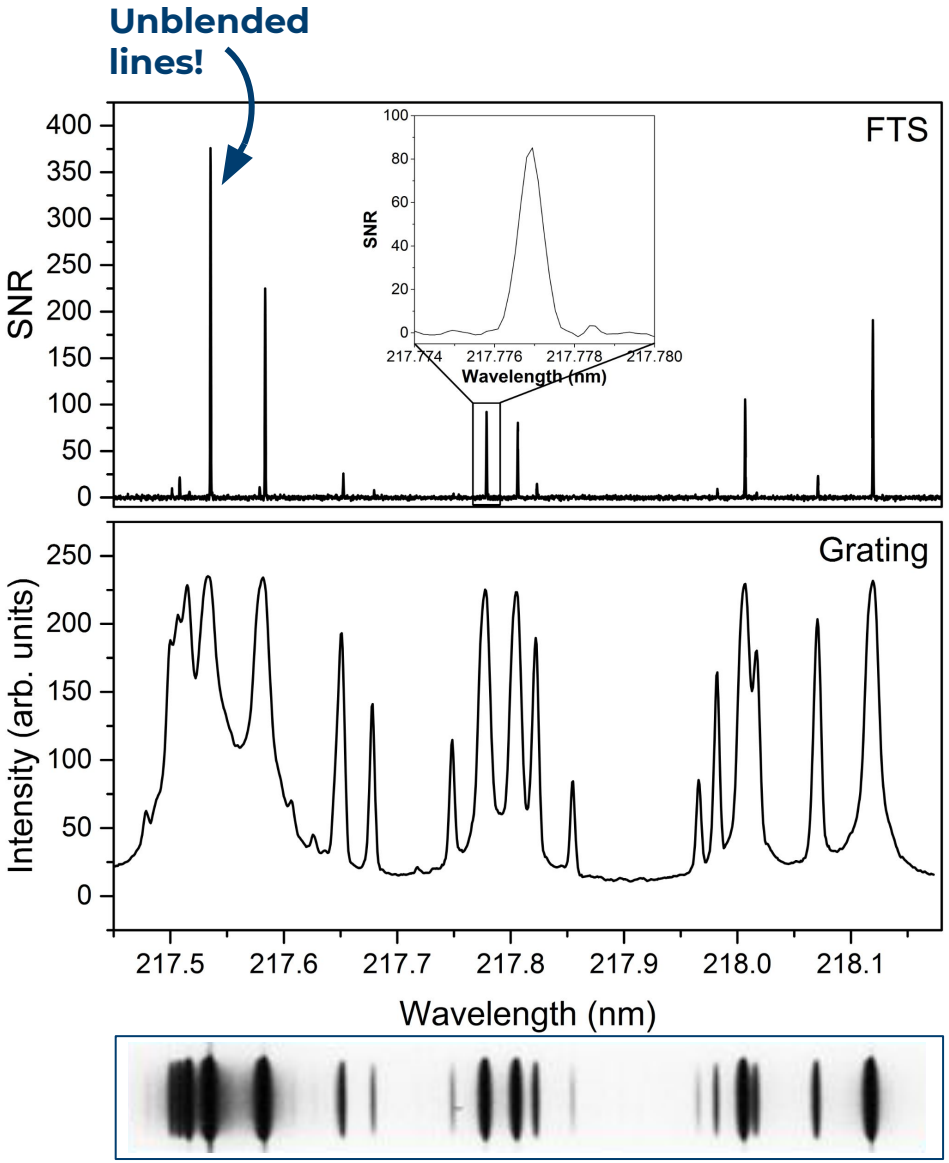
The FTS uses **stable** light sources, such as the Hollow Cathode Lamps for neutral atoms and singly-ionised ions, and the Penning Discharge Lamp for doubly-ionised ions.

We intensity calibrate using tungsten and deuterium standard lamps.

[1] Nature Editorial, 503/7477, 437 (2013)

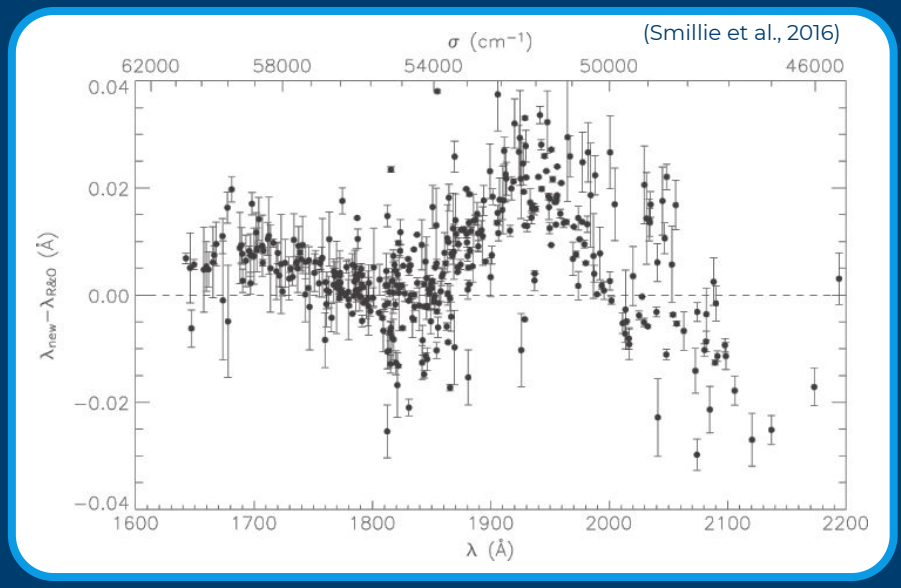
FTS vs Grating Spectra

FTS improves accuracy of wavelengths and energy levels by at least an order of magnitude over previously used Grating Spectroscopy.

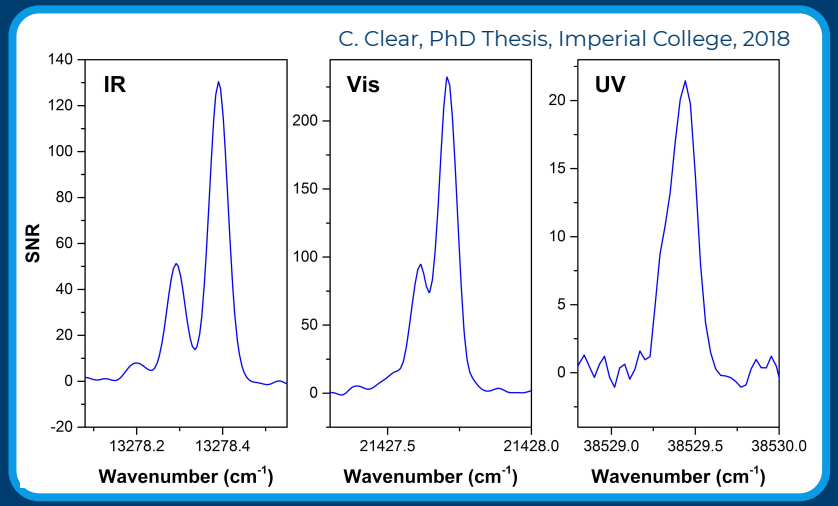


C. Clear, PhD Thesis, Imperial College, 2018

Below is an example of wavelength accuracy improvement between our FTS measured **Co III** wavelengths and those from Raassen & Ortin (1984) grating spectra [2]. Error bars are the combined uncertainties, predominantly from the grating data. Wavelength differences exceed the grating spectra uncertainty (10 mÅ), showing the inaccuracies of the past grating data.



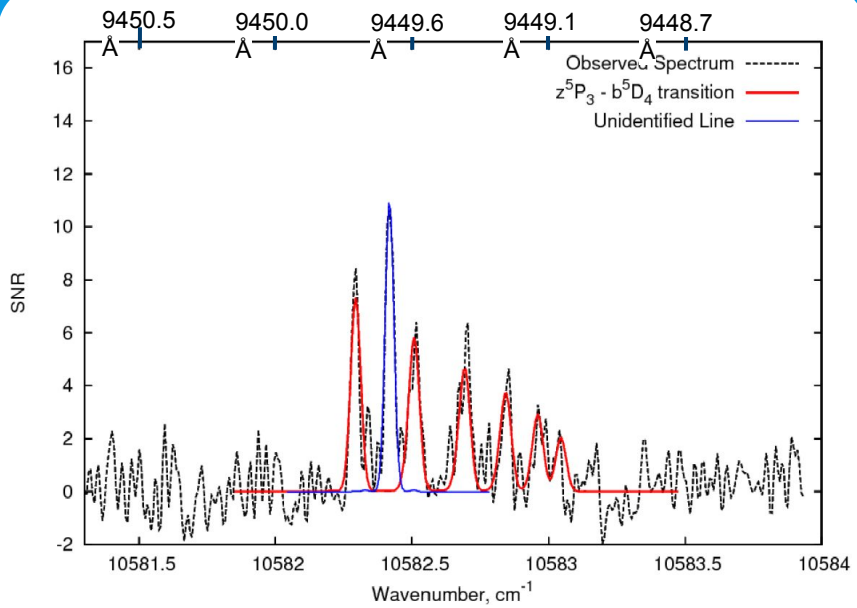
The FTS also resolves lines to show **isotope structure**. Below is an example of isotope structure in Ni II [$3d^74s^2$ - $3d^8$ (^{3}F)4p] in the IR, visible and UV spectral regions.



[2] Smillie, Pickering, Nave, & Smith, 2016. ApJSSeries, 223(1):12.

We use our accurate FTS measured wavelengths to improve energy levels (uncertainty up to 0.001 cm^{-1}) and search for unknown energy levels [3,4]. We improve previously classified levels and lines by at least an order of magnitude.

Data for neutral, singly and doubly ionised **iron-group elements** are urgently required. These elements have a complex atomic structure, resulting in many spectral lines from the VUV to IR. They account for the majority of opacity in stars due to relatively high abundances and large number of energy levels.



The hyperfine-split profile of the z^5P_3-b^5D_4 transition in **Mn II**, as observed (black) and fitted (red).

F.Liggins, PhD Thesis, Imperial College, 2018

[3] Thorne, Pickering, Semeniuk, ApJSSeries. 2010;192(1):11.
[4] Thorne, Pickering, Semeniuk, ApJSSeries. 2013;207(1):13.
[5] Liggins, Pickering, Nave, Ward, and Tchang-Brillet, ApJSSeries. 2021;252(1):10.
[6] Liggins, Pickering, Nave, Kramida, Gamrath, and Quinet, ApJSSeries. 2021;907(2):69.
[7] Ding M and Pickering J, ApJSSeries. 2020; 251(2):24.
[8] Smillie, Pickering, & Smith, MNRAS. 2008;390(2):733.

The IC group have studied singly ionised iron-group elements, including **Ti II**, **V II**, and **Fe II.** Most recently, we have published data for **Mn II** [5,6], **Co II** (HFS analysis)[7] and **Ni II** (Clear et al., 2021, *in preparation*).

Recent work on the doubly ionised iron-group elements includes:

- **Cr III**, first high resolution measurements of UV transition wavelengths, which are used as wavelength standards published [8].
- **Co III**, order of magnitude improvement in wavelengths and energy levels. [2]
- **Fe III**, new spectra have been recorded in the VUV, providing accurate wavelengths with a new energy level analysis almost complete.

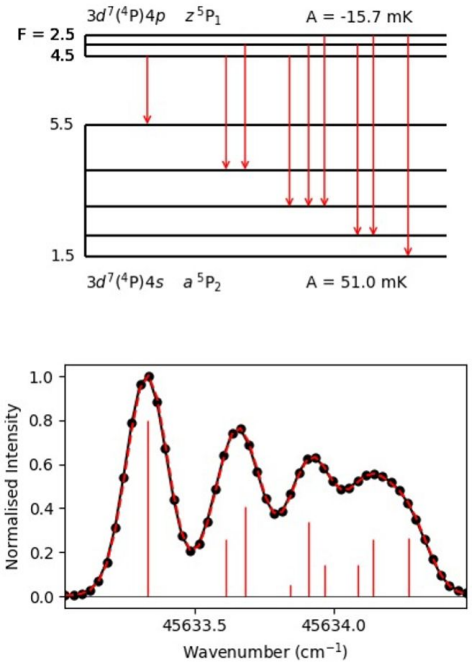
*Analysis is also in progress for **Mn I** to give accurate wavelengths and energy levels.*

Accurate **Hyperfine structure** (HFS) data are vital for chemical abundance determinations and line identifications. Lines broadened due to hyperfine components could easily be interpreted as many lines.

HFS is present, for example, in manganese and cobalt spectra. In the **Mn II** example to the left, the previously published wavenumber will have been dominated by the unidentified line blended with this transition.

We analysed the HFS constants of **Co II**, fitting over 700 spectral lines, leading to measurements of 292 magnetic dipole hyperfine interaction A constants, (increasing the number of **Co II** levels with known A values tenfold!) [7].

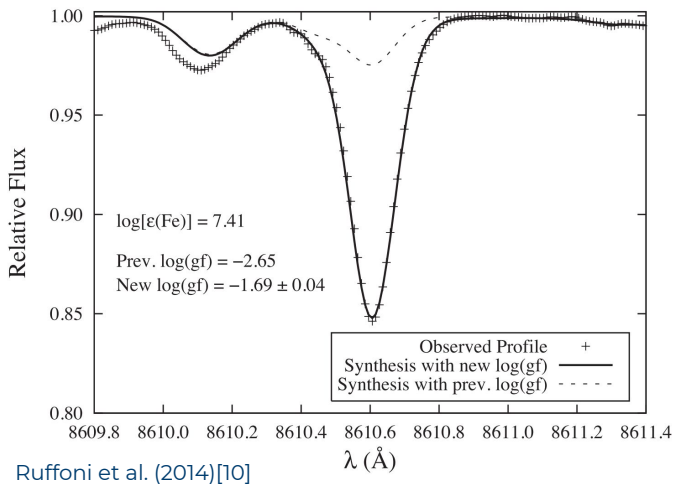
HFS Fitting of Co II lines



Oscillator strengths (or log(gf)s) are also required, ideally to 10% accuracy or better, as they are essential in abundance calculations.

There have been improvements in **Fe I** [9,10,11,12], **Fe II** [13,14], **Sc II** [15], **V I** [16], **Mn I** [17,18], **Ti I** [19] and **Ti II** [20]. Below is an example of an **Fe I** line observed in the solar spectrum and synthesized using both the log(gf) values from Ruffoni et al. (2014)[10] and the best previously published value.

*Analysis is in progress for **Mn II** log(gf)s.*



Ruffoni et al. (2014)[10]

[9] Ruffoni, Allende Prieto, Nave, & Pickering, ApJ. 2013;779(1):17.
[10] Ruffoni, Den Hartog, Lawler, Brewer, Lind, Nave, & Pickering, MNRAS. 2014;441(4):3127.
[11] Den Hartog, Ruffoni, Lawler, Pickering, Lind & Brewer, ApJSSeries. 2014;215(2):23.
[12] Belmonte, Pickering, Ruffoni, Hartog, Lawler, Guzman, & Heiter, ApJ. 2017;848(2):125.
[13] Pickering, Johansson, & Smith, A&A. 2001;377(1):361
[14] Pickering, Donnelly, Nilsson, Hibbert, & Johansson, A&A. 2002.;396(2):715-722.
[15] Pehlivan Rhodin, Belmonte, Engström, Lundberg, Nilsson, Hartman, Pickering, Clear, Quinet, Fivet, V. & Palmeri, MNRAS. 2017;472(3):3337
[16] Holmes, Pickering, Ruffoni, Blackwell-Whitehead, Nilsson, Engström, Hartman, Lundberg, Belmonte, ApJSSeries. 2016;224(2):35.
[17] Blackwell-Whitehead, Xu, Pickering, Nave, & Lundberg, MNRAS. 2005;361(4):1281
[18] Blackwell-Whitehead, Pavlenko, Nave, Pickering, Jones, Lyubchik, & Nilsson, A&A. 2011;525:A44.
[19] Blackwell-Whitehead, Lundberg, Nave, Pickering, Jones, Lyubchik, Pavlenko, & Viti, MNRAS. 2006;373(4):1603
[20] Pickering, Thorne, & Perez, ApJSSeries. 2001;132(2):403-409.
[21] Nave, & Clear, MNRAS. 2021;502(4):5679

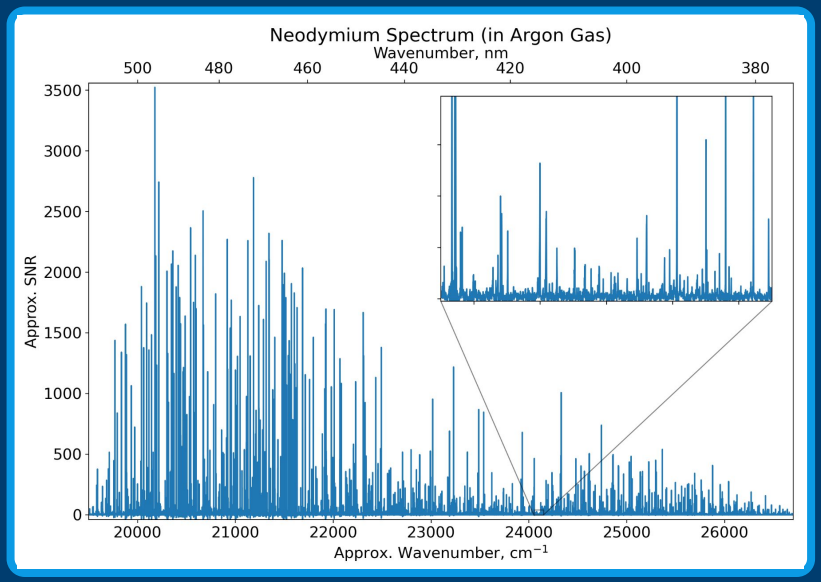
Applications of atomic data include the identification of lines, disentangling of blends and creating synthetic stellar spectra. To analyse astrophysical spectra, state-of-the-art stellar atmosphere models rely on atomic data from every element that may contribute to the spectrum, therefore a thorough atomic database is needed.

A wide range of accurate atomic data is required for Galactic Surveys (APOGEE, Gaia-ESO Survey, WEAVE, etc.), which are interested in obtaining chemical abundances for different elements including iron-group and some lanthanide elements.

Measurements have also been used to better analyse quasar spectra, to constrain space-time variations in the fine structure constant α [21].

We take requests!

Please contact us with any specific data needs. We are developing a defined list of anticipated needs.



Due to requests, the study of **Nd II** & **Nd III** is in progress at Imperial College. Left is an example of the very dense neodymium spectrum recorded on the FTS.

Atomic data for **lanthanide elements** are required to decipher kilonova produced by the merging of compact binary star systems and to study chemically peculiar stars.

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