

# Atomic structure and collisional data for heavy elements $Z \geq 50$ involved in Neutron Star mergers: Dr C Ballance and Dr C Ramsbottom

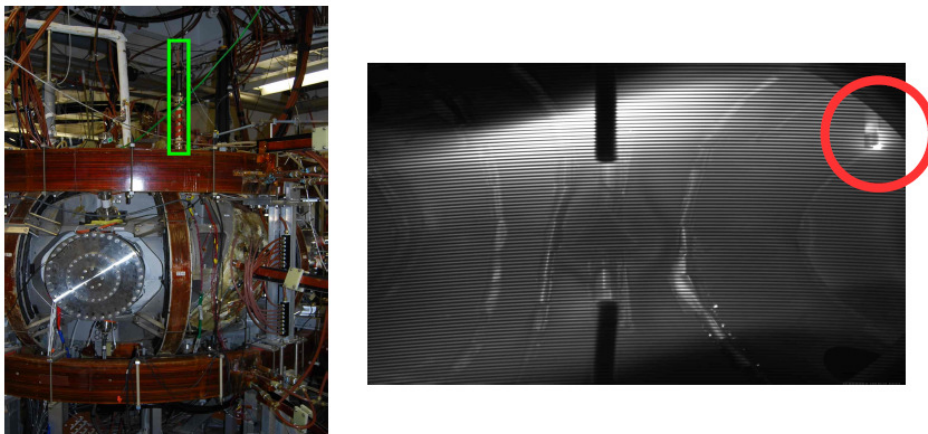
With the advent of detecting gravitational waves from a binary neutron star merger (NSM) by the LIGO collaboration and follow up studies of the electromagnetic counterpart(s), interest in heavy  $r$ -process elements has increased dramatically. Immediately following a NSM, physical conditions are expected to produce significant abundances of  $r$ -process elements, including the lanthanides, actinides, and platinum-group elements. Given their expected contributions to NSM spectra, both AMO theorists and experimentalists have received increasing demand to determine spectral emission and atomic data for these elements.

The approach to this project is two-fold: Theoretically at QUB, Drs Ballance and Ramsbottom maintain and develop relativistic atomic structure and electron/photon collisional codes that underpin collisional radiative models that may be used to interpret such observed spectra. Secondly, our colleagues at Auburn University maintain several plasma experiments i.e. the large Compact Toroidal Hybrid (CTH) (see below) and various Hollow Cathode Discharge tubes with filaments of Gold, Platinum and Iridium which produce spectral lines of interest in the UV.

One of the issues of the NIST database, beyond providing the energy levels and Einstein A-coefficients for the neutral species is that they are lacking detailed information for near-neutral systems up to doubly ionized cases. We are proposing comprehensive atomic structure calculations for Tin (Sn) and Osmium (Os) to compliment recently published work on Gold (Gillanders 2021[1], McCann 2021[2]). Preliminary collisional calculations reveal that the first few metastables are not in Local Thermal Equilibrium (LTE) and therefore collisional calculations may be required.

## 0.1 Plan of work

The project shall proceed as follows. There shall be a review of the atomic structure, the underlying electron-impact driven collisional processes as well as collisional-radiative theory. We shall calculate everything needed from first principles using the R-matrix suite of collisional codes. Collisional radiative models will be built from these results. There is the opportunity to run these calculations on National supercomputers both within the US and Europe. A large aspect of the project, shall be the interaction with the Auburn University experimental group to match and identify lines observed from their experiments.



**Figure 1.** Compact Toroidal Hybrid Experiment at Auburn University. This magnetically-confined plasma device is approximately 10 feet high, with various diagnostic ports across the circumference. On the top left-side of the figure, the infra-red diagnostic port is highlighted by the green rectangle. The right picture illustrates a small block of Tungsten  $Z = 74$  introduced into the plasma, radiating under normal operating conditions.

## 0.2 Background

It would be beneficial if the prospective student has an entry-level quantum mechanical course. There is the intent that the student would calculate all the atomic processes required to develop, with guidance, their own collisional-radiative models. Therefore, some basic understanding of numerical methods as implemented with either Matlab, C++ , Fortran or their more modern equivalents would be desirable. However, more important is an interest in the topic as these skill-sets can be acquired during the project.

### 0.3 Aims and objectives of the project

- To provide the student with a complete survey of the collisional processes involved with plasma collisional-radiative modelling. To take first principle atomic calculations through to interpretation of spectra.
- There is a strong computational aspect, therefore an interest in computational modelling, and in particular utilizing powerful parallel supercomputers is required.
- There will be a strong collaboration between experimental groups in the US and researchers at Queens. Identifying strong spectral lines observed from various experimental devices under particular temperature and density conditions shall be an integral part of the project. However, theoretically, collisional radiative modelling should allow us to be more proactive in suggesting diagnostic lines for the experimental groups to observe.
- The Phd student should be prepared to spend short periods at Auburn University and to present their work and relevant astrophysical and atomic physics conferences.
- To acquire good programming and numerical skills valuable for graduate level work, which are also marketable skills within the workplace.

### References

[1] Constraints on the presence of platinum and gold in the spectra of the kilonova AT2017gfo

J H Gillanders, M McCann, S A Sim, S J Smartt, C P Ballance

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[2] Atomic data calculations for Au i–Au iii and exploration in the application of collisional-radiative theory to laboratory and neutron star merger plasmas

Michael McCann, S Bromley, S D Loch, C P Ballance

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