Geant4 X-ray fluorescence with ANSTO library

S. Bakr[1], D.D. Cohen[2], R. Siegele[2], J. Archer[1], S. Incerti[3,4], V. Ivanchenko[5,6], A. Mantero[7], A. Rosenfeld[1], S. Guatelli[1,8]

1. CMRP, University of Wollongong, Australia
2. Australian Nuclear Science and Technology Organization
3. CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux-Gradignan
4. Université de Bordeaux, Centre d'Etudes Nucléaires de Bordeaux-Gradignan
5. Geant4 Associates International Ltd
6. Tomsk State University, Russia
7. SWHARD s.r.l.
8. Illawarra Health and Medical Research Institute, University of Wollongong, NSW, Australia

Goal of the project

Develop a new library, called here ANSTO, modelling PIXE (p and α cross sections and fluorescence) based on the approach described in [*].

- Thoroughly validated against experimental measurements performed at ANSTO.
- Cross sections up to 5 MeV/u
- Alternative to the existing Geant4 PIXE and fluorescence data libraries

* D. D. Cohen, et al. “K, L, and M shell datasets for PIXE spectrum fitting and analysis,” Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms, vol. 363, pp. 7–18, 2015

PIXE in Geant4

Currently three PIXE cross sections data sets in Geant4:

1. **Empirical**, K and L shell ionisation cross

2. **Analytical**, based on the ECPSSR theory for the description of K and L shells ionisation for incident protons and α particles.

3. **ECPSSR Form Factor**, based on a polynomial approximation of the ionisation cross sections of K, L and a selection of M shells calculated by Taborda et al (Incerti, Barberet et al. 2015)

4. **ANSTO ECPSSR**, cross sections for incident proton and alpha particles to be integrated in Geant4 for PIXE simulation.


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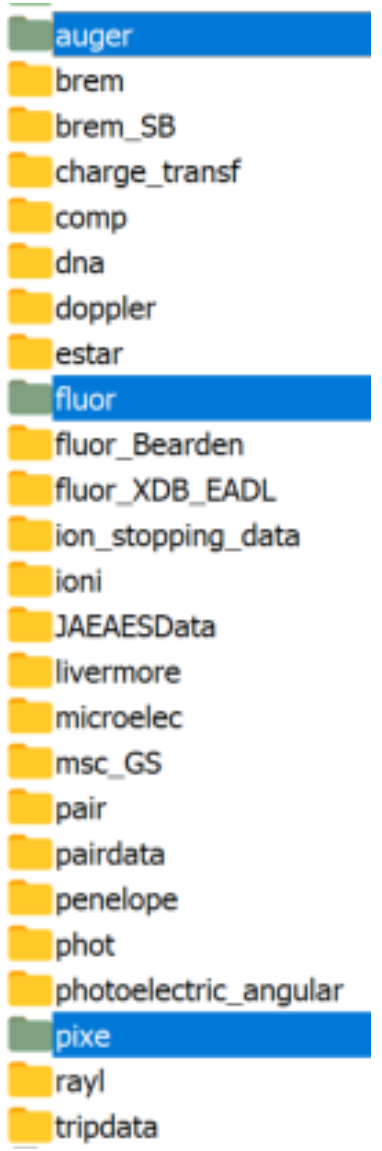
Latest Geant4 developments for PIXE applications

S. Bakr[a,*], D.D. Cohen[b], R. Siegele[b], S. Incerti[c,d], V. Ivanchenko[e,f], A. Mantero[g], A. Rosenfeld[a,h], S. Guatelli[a,h]

[a] CMRP, University of Wollongong, Australia
[b] Centre for Accelerator Science, Australian Nuclear Science and Technology Organization, Australia
[c] CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux-Gradignan, France
[d] Université de Bordeaux, Centre d'Etudes Nucléaires de Bordeaux-Gradignan, France
[e] Geant4 Associates International Ltd, United Kingdom
[f] Tomsk State University, Russia
[g] SWHARD s.r.l, Italy
[h] Illawarra Health and Medical Research Institute, University of Wollongong, NSW, Australia

PIXE in Geant4

G4EMLOW



1. The **creation of a vacancy** in a sub/shell.

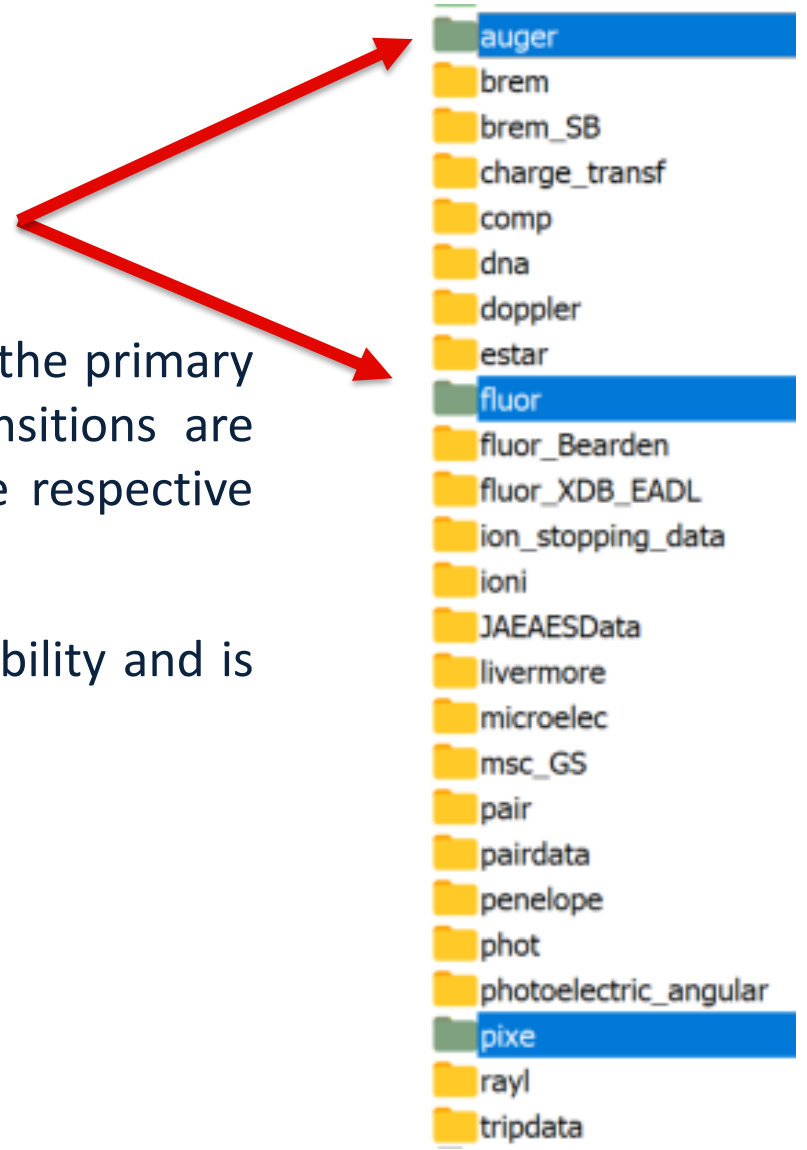
Two ionisation cross-section models have been used in this work:
a) ECPSSR form-factor: a polynomial approximation of the ionisation cross sections of K, L and M shells.

b) ANSTO: based on the ECPSSR approach of the ionisation cross sections of K, L and M sub/shells as calculated by D.D. Cohen et al for incident protons and alpha particles

- PIXE ionisation cross sections

PIXE in Geant4

G4EMLOW



2. Then the **relaxation** cascade is triggered

The relaxation cascade is triggered, starting from the vacancy created by the primary process. Fluorescence X-ray or Auger electrons and Coster-Kronig transitions are generated through radiative and non-radiative transitions, based on the respective transition probabilities.

EADL is the library that is used in Geant4 to provide the transition probability and is based on Hartree-Slater approach.

- EADL* libraries

- Perkins ST, Cullen DE, Chen MH, Rathkopf J, Scofield J, Hubbell JH.
  Tables and Graphs of Atomic Subshell and Relaxation Data Derived from the LLNL Evaluated Atomic Data Library,
  ${Z}=1-100$. *Eadl*. 1991;30:UCRL-50400. doi:10.2172/10121422

EADL and ANSTO data libraries: Comparison

We are comparing Geant4 results using

Ionisation cross-sections models	Transition probabilities
Form Factor-ECPSSR [4-5]	EADL (Hartree-Slater)
ANSTO	extracted from ANSTO data

- ionisation cross-sections:
  - Based on Form Factor (Taborda K, L, M 2011-2013)
  - ANSTO PIXE cross section

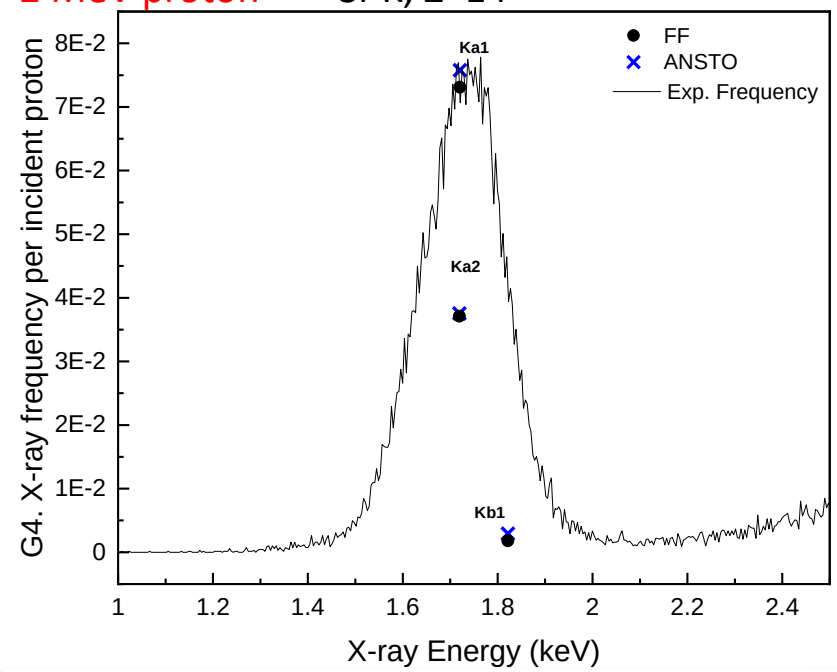
- Transition probabilities:
  - EADL, G4EMLOW7.7
  - ANSTO-fluo
    - D. D. Cohen, J. Crawford, and R. Siegele, “K, L, and M shell datasets for PIXE spectrum fitting and analysis,” Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms, vol. 363, pp. 7–18, 2015.
    - Data library of ANSTO with the same format of EADL (G4EMLOW7.7/fluo)
    - The same binding energies of EADL are adopted
  - The radiative transition probabilities reported in the EADL were calculated according to Hartree Slater (HS) methods, however [Cohen et al 2015] recommends the Hartree-Fock approach for M shell

Methodology

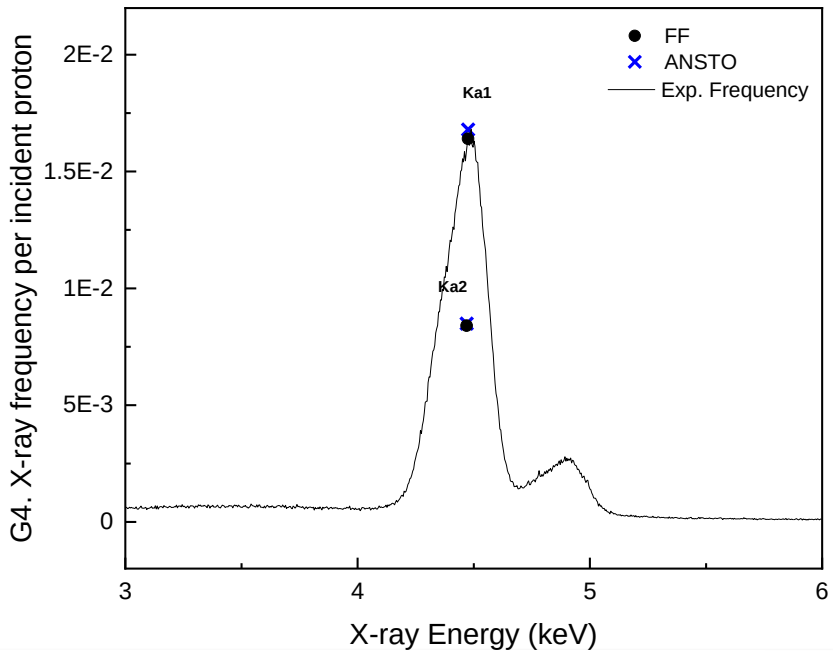
- **Geant4 TestEm5 extended example (Geant4 10.05.p01)**
  - Monochromatic beams of proton and alpha particles are incident on 25 µm thick targets (50 µm lateral sizes).
  - The new data library, ANSTO, same format of the existing EADL Geant4 data library.
  - ANSTO and EADL, has been quantified in terms of fluorescence X-ray yields per incident particle.

2 MeV proton

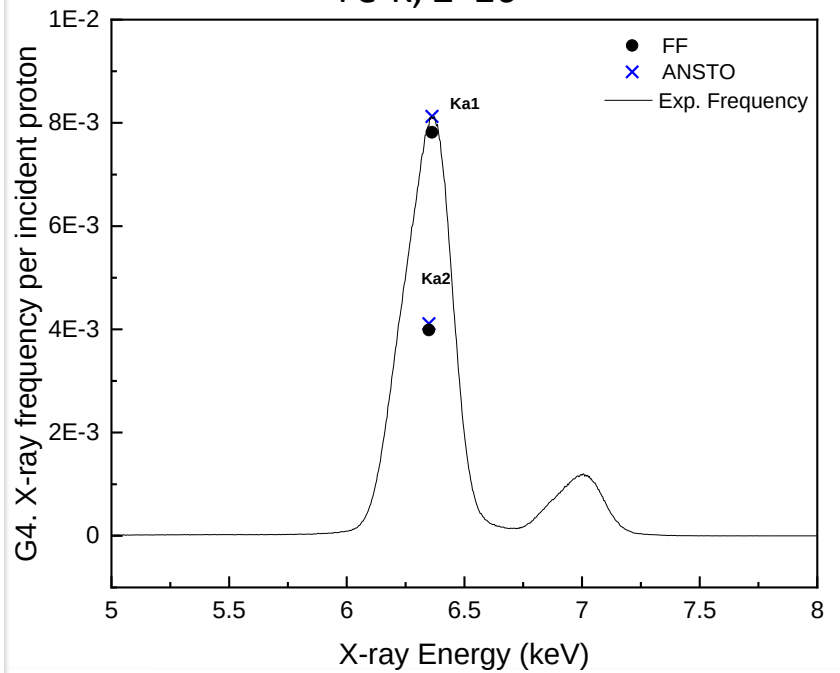
Si-K, Z=14



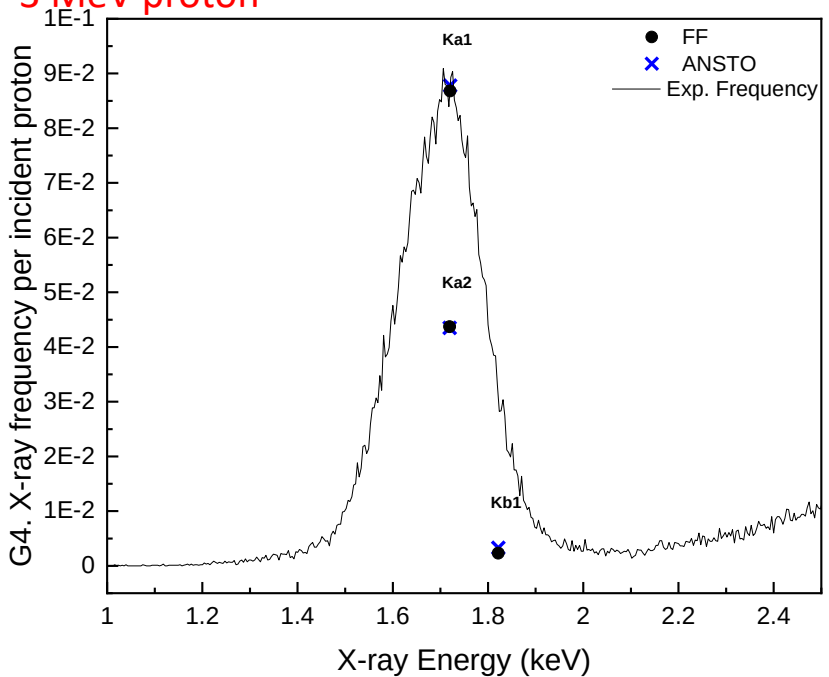
Ti-K, Z=22

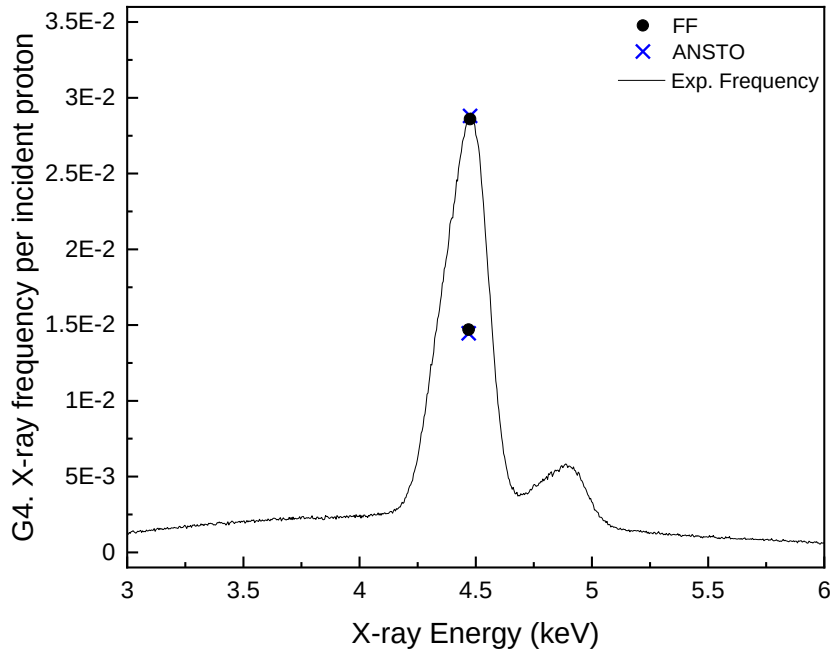


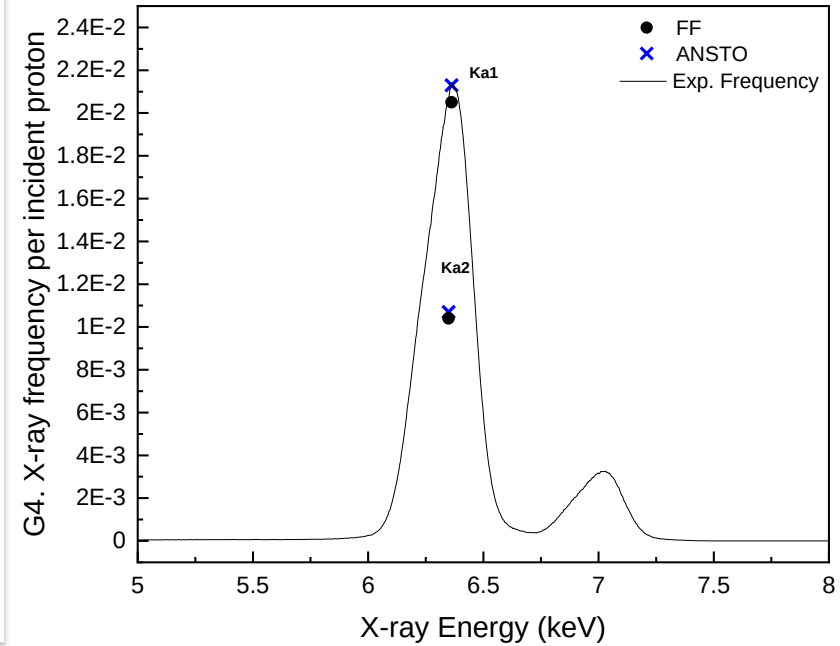
Fe-K, Z=26



3 MeV proton

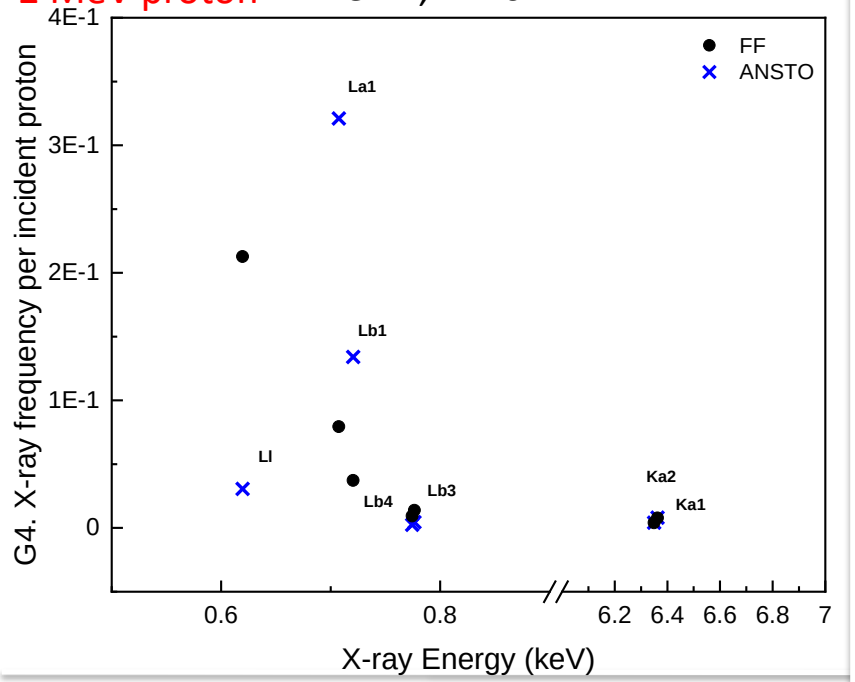




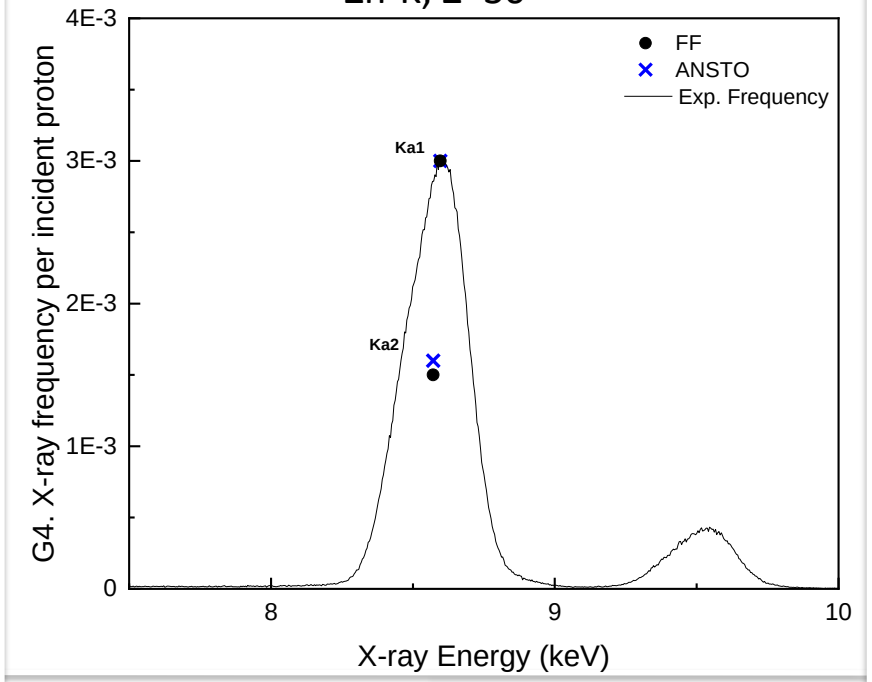


2 MeV proton

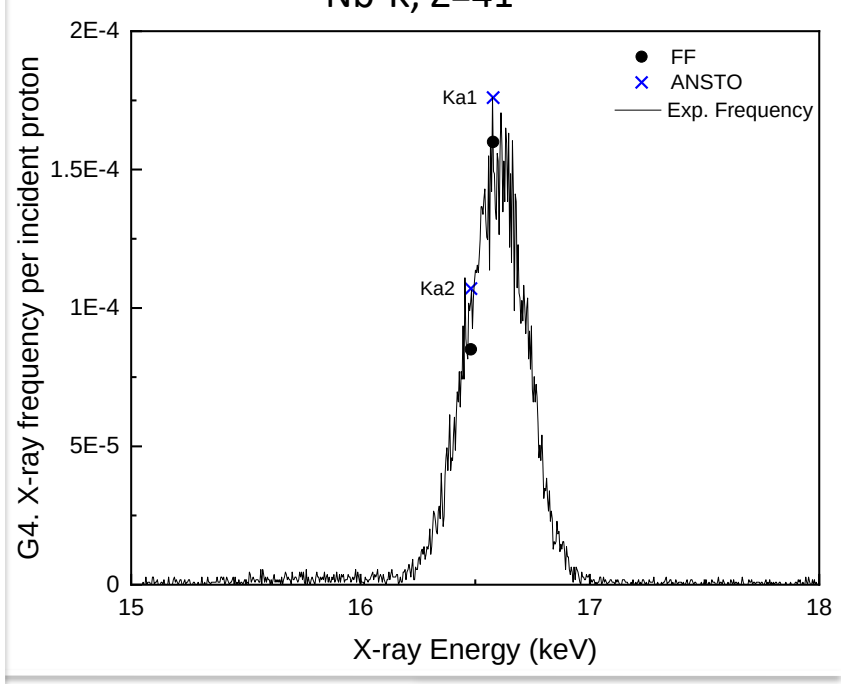
Fe-KL, Z=26



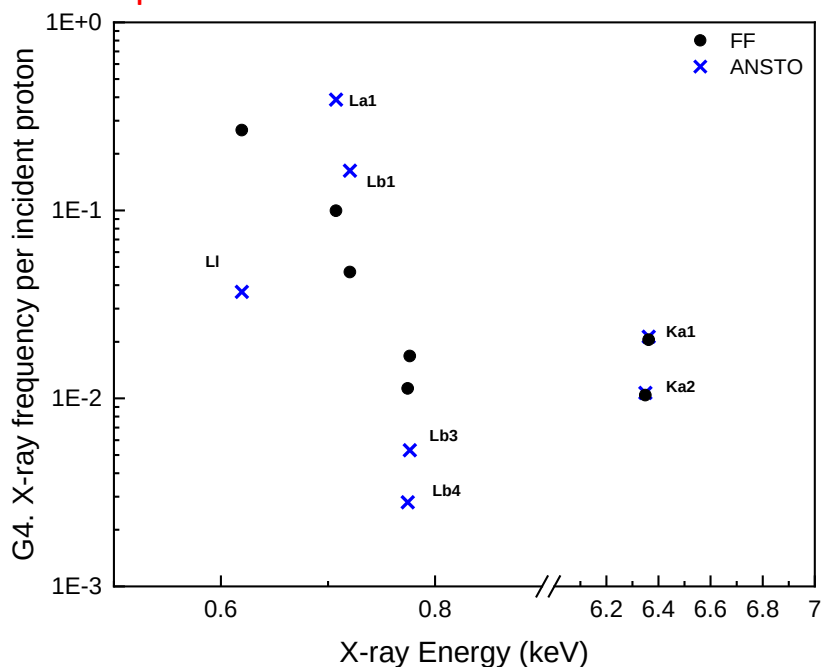
Zn-K, Z=30

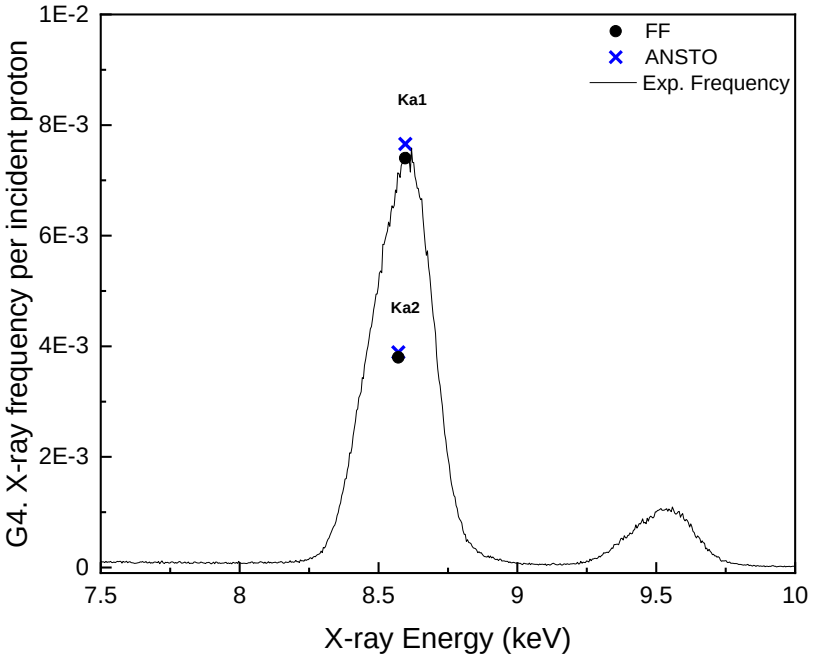


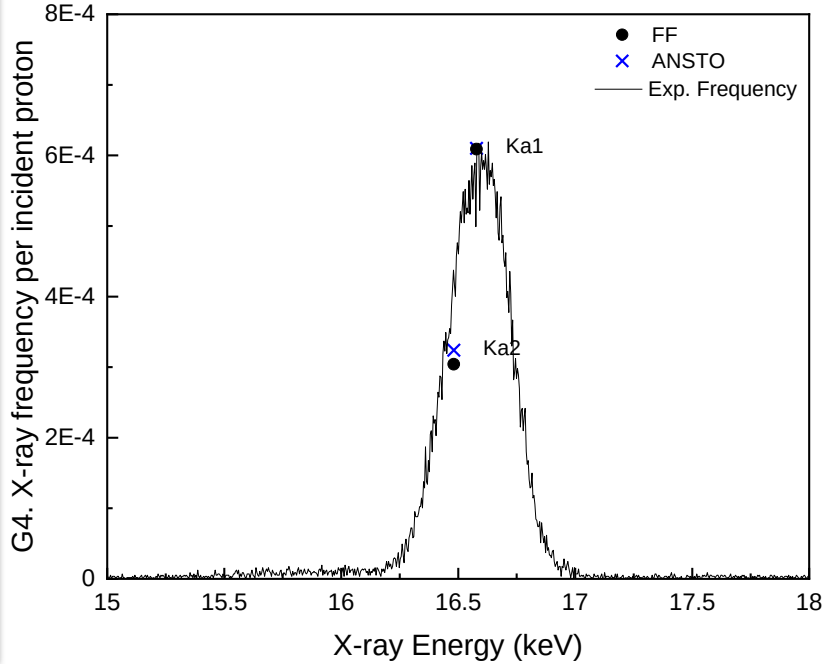
Nb-K, Z=41



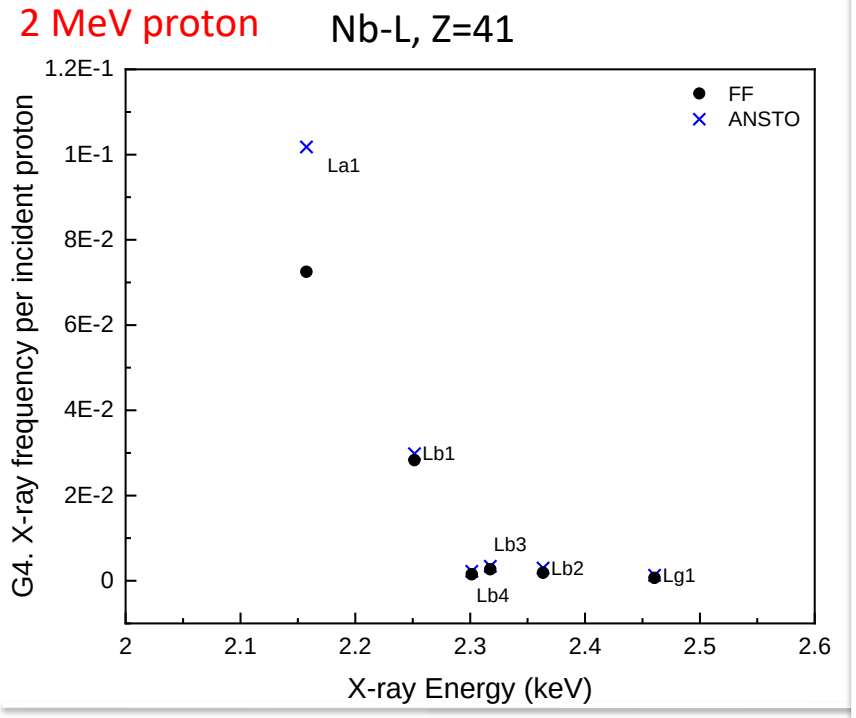
3 MeV proton

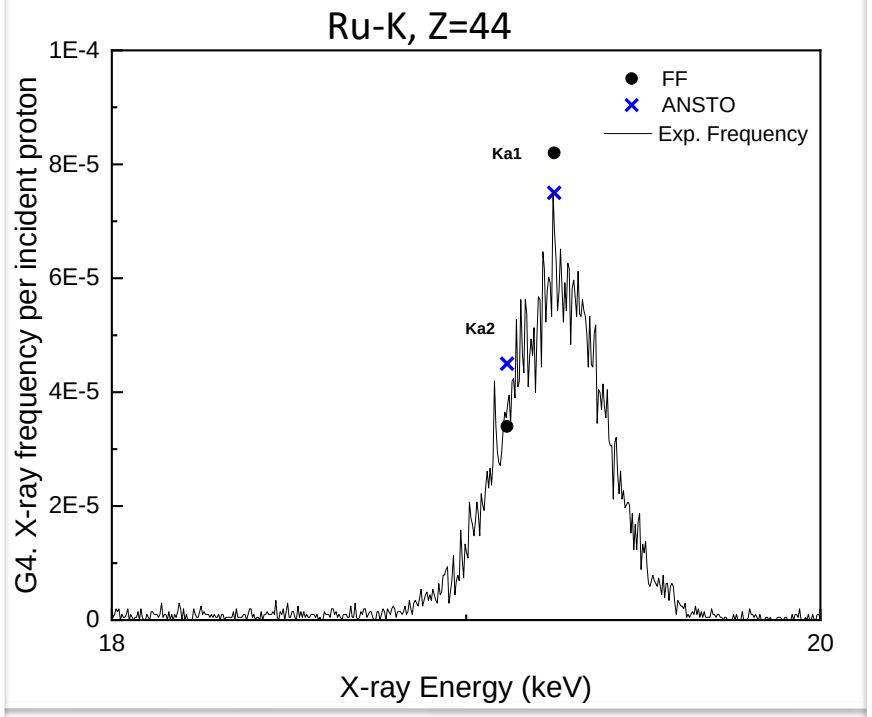


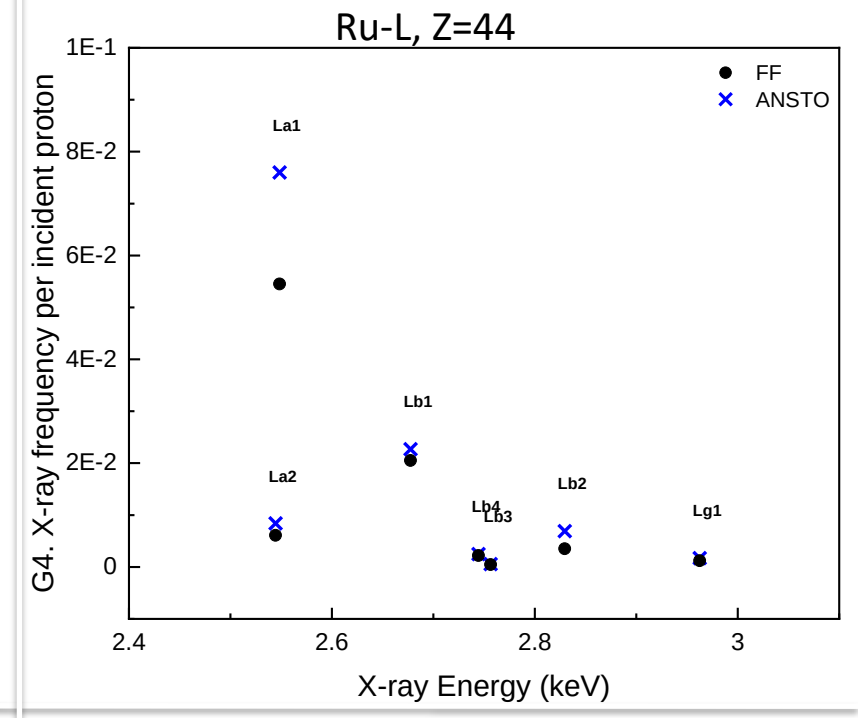




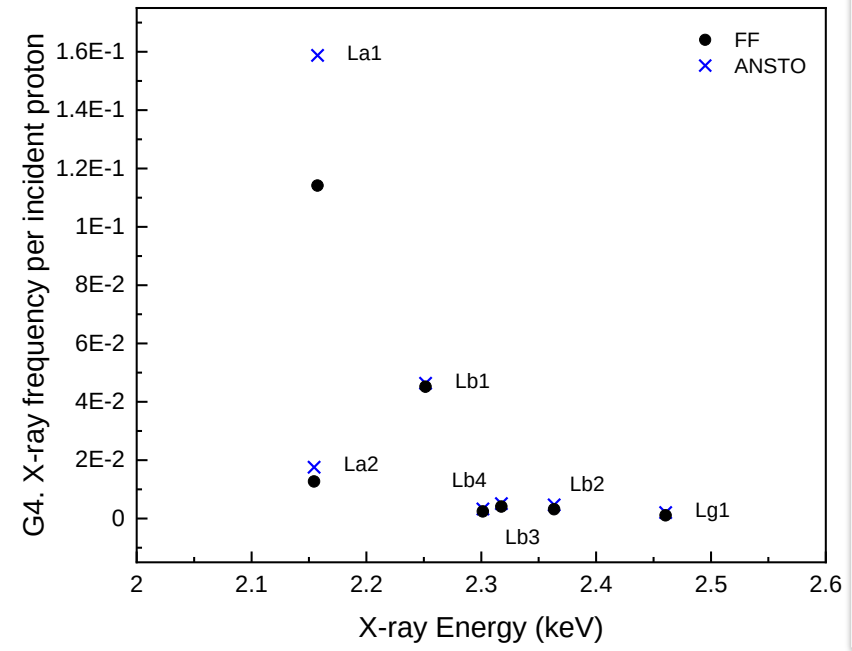
2 MeV proton

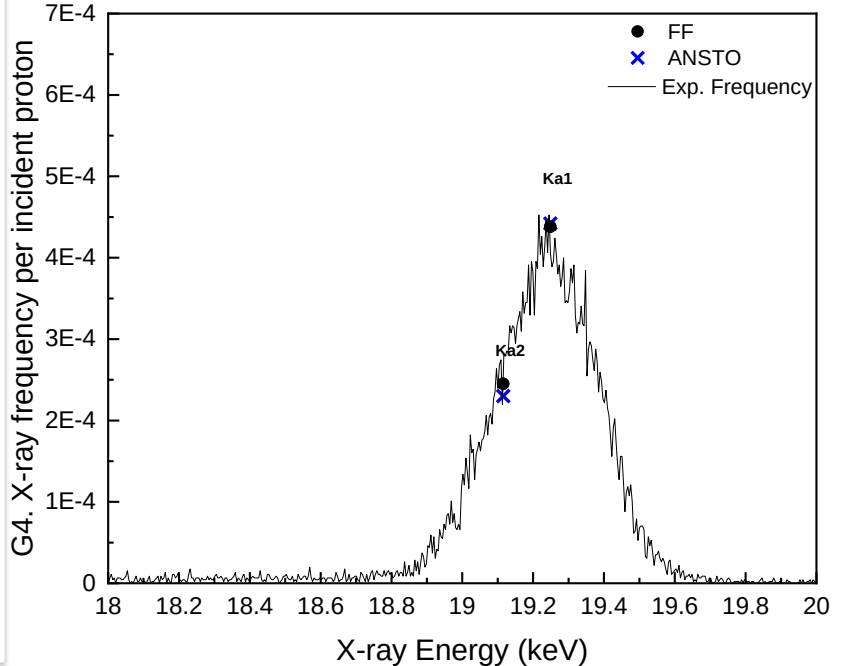


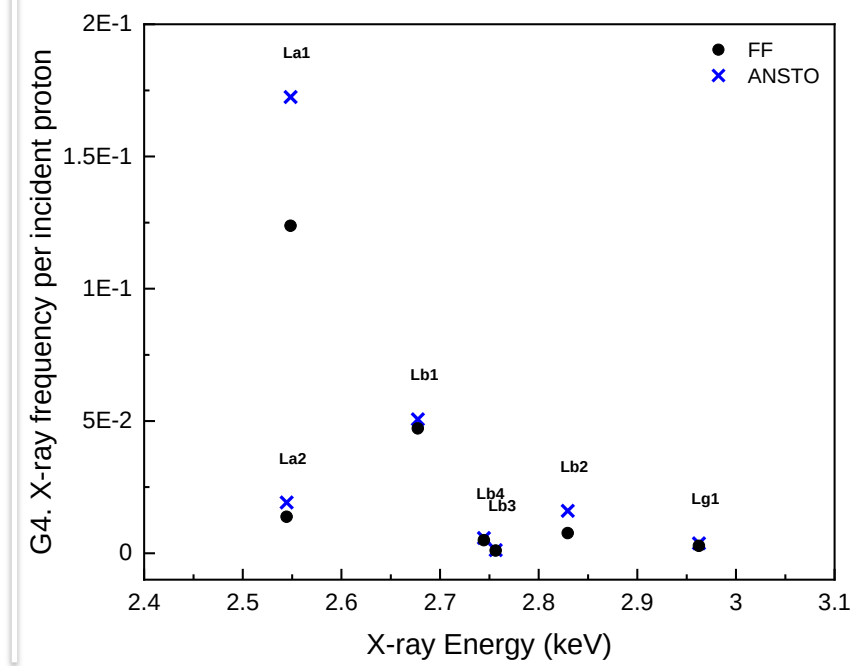




3 MeV proton

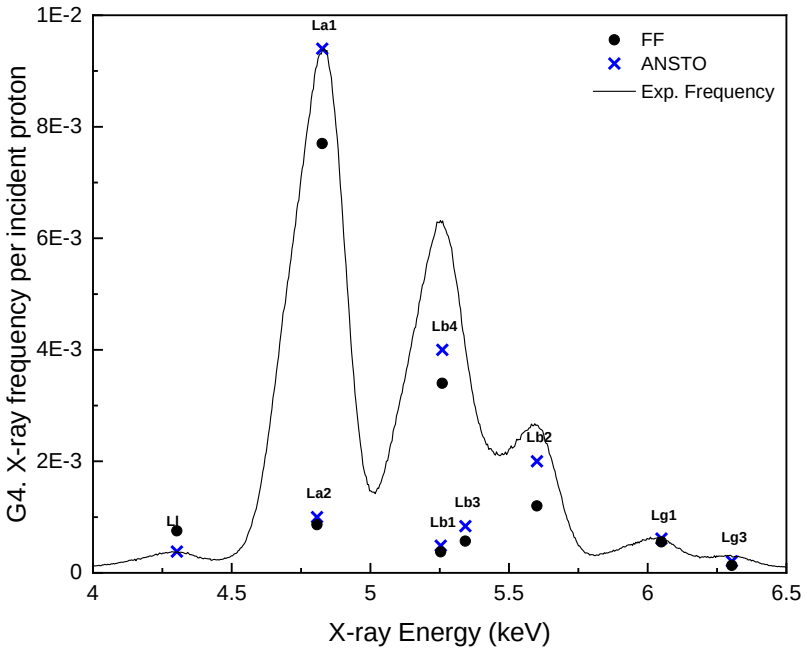




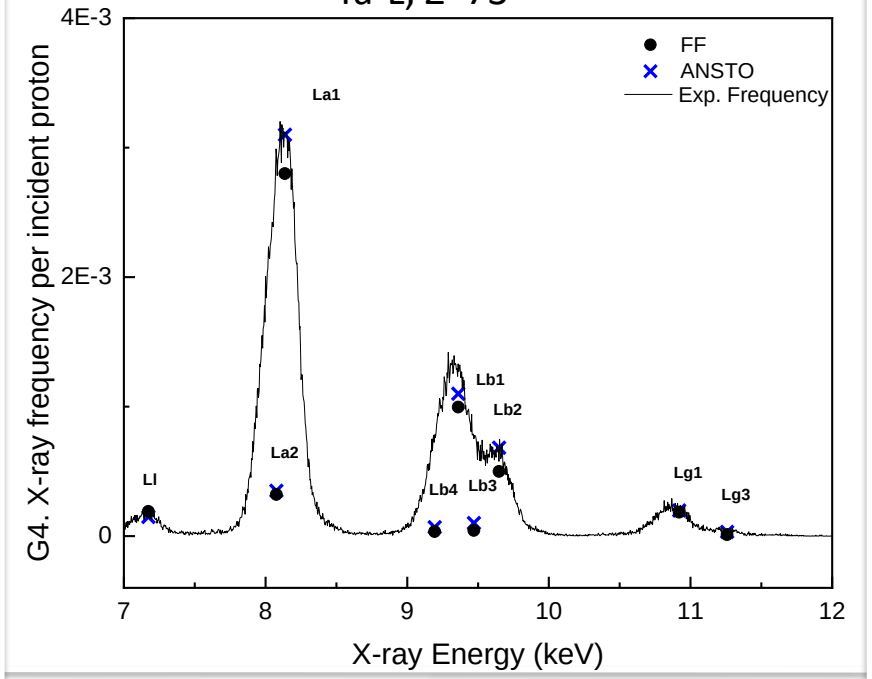


2 MeV proton

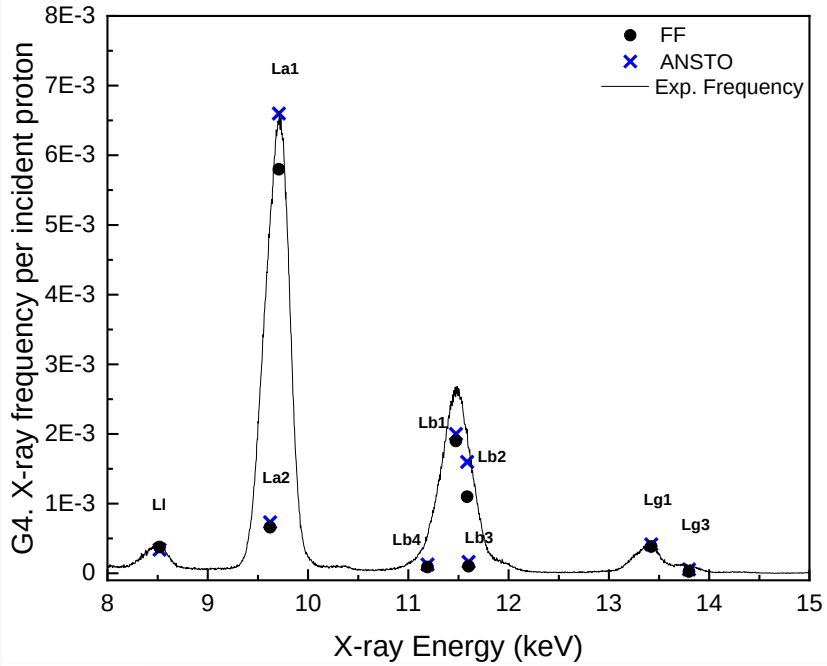
Ce-L, Z=58



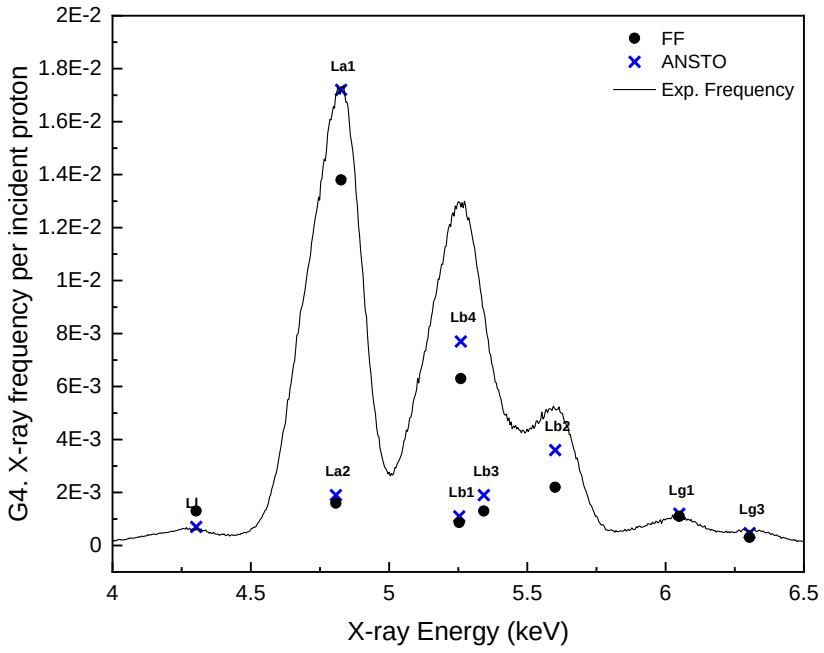
Ta-L, Z=73

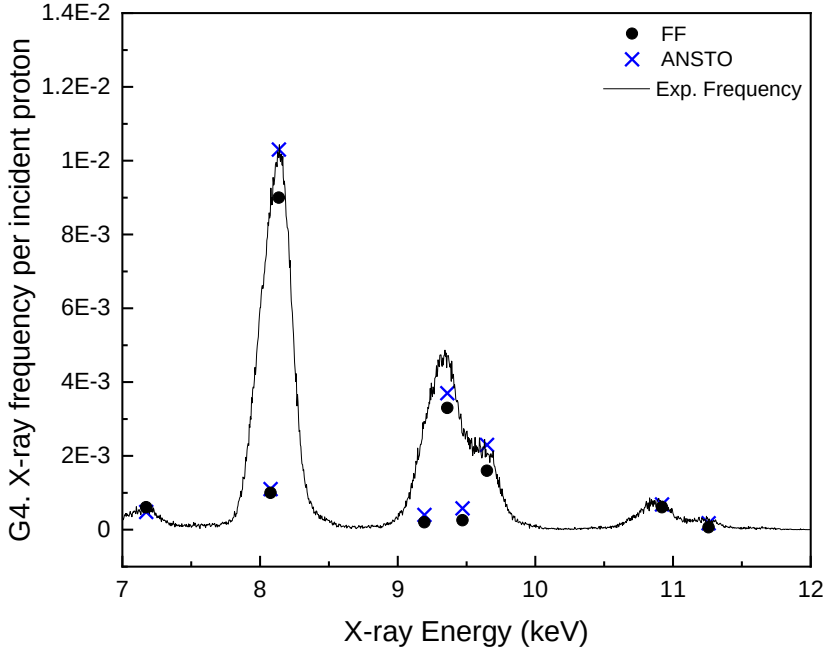


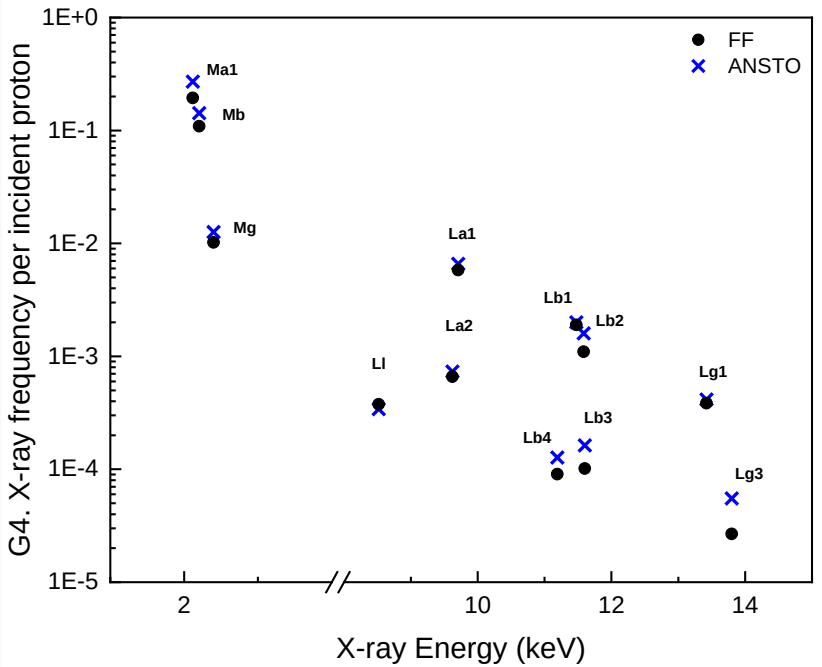
Au-L, Z=79



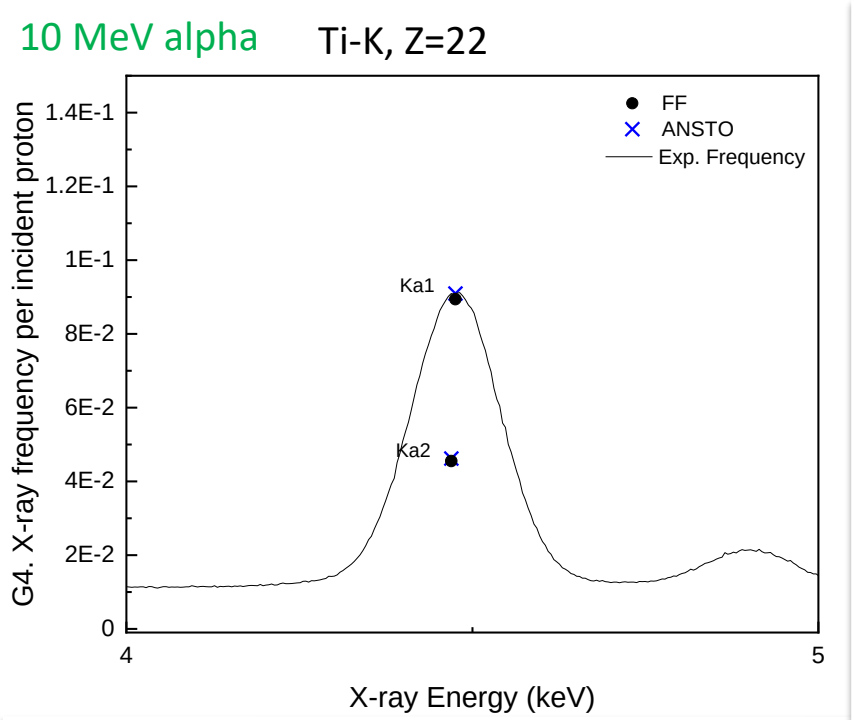
3 MeV proton

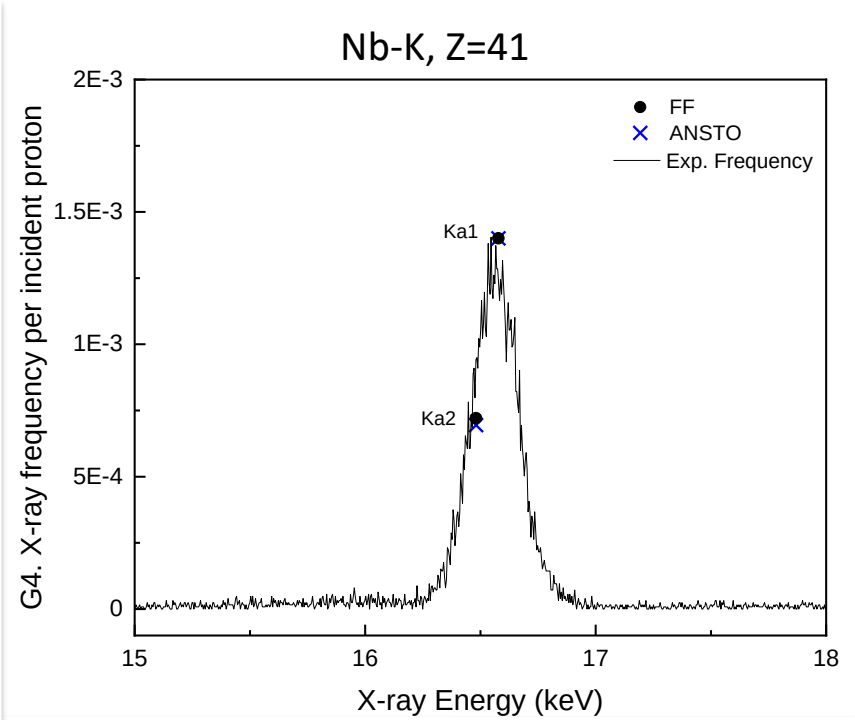


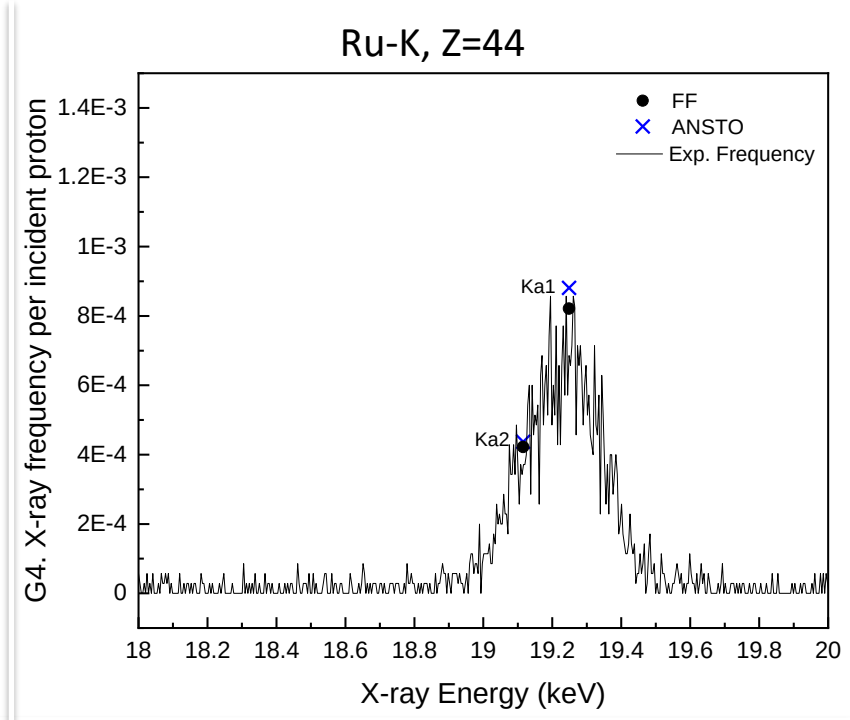


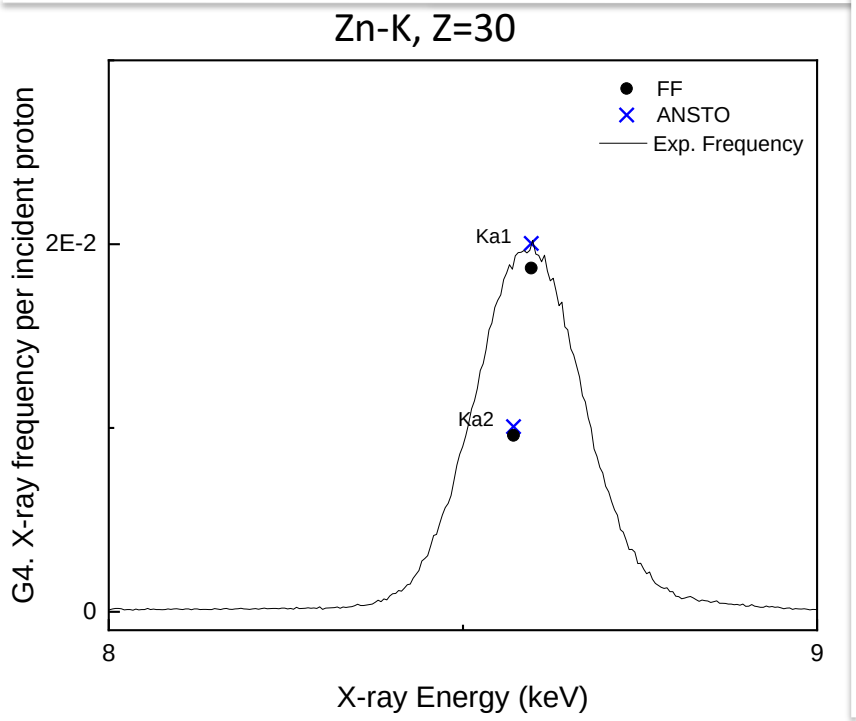


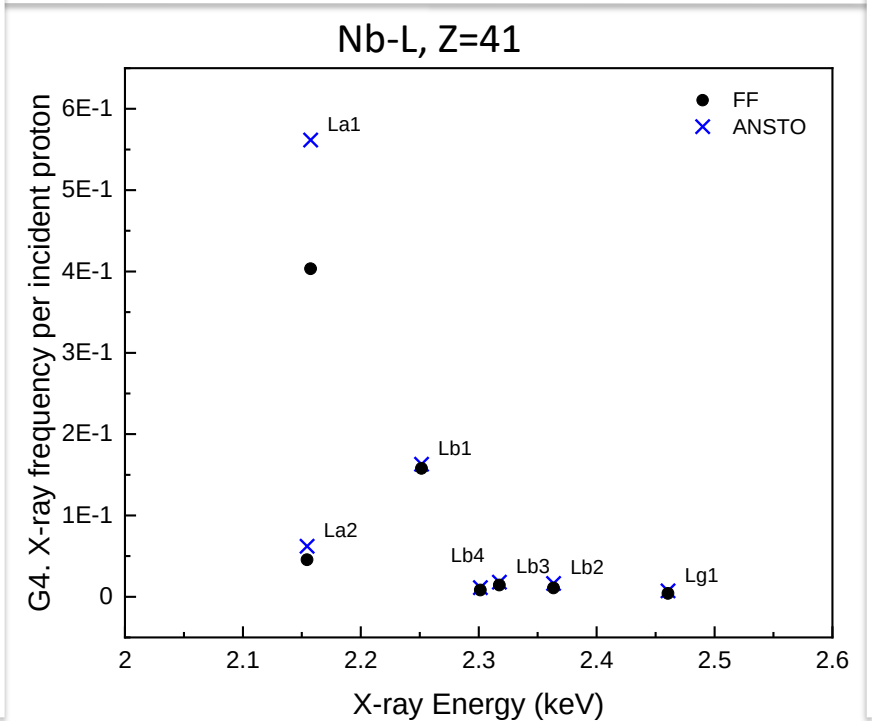
10 MeV alpha

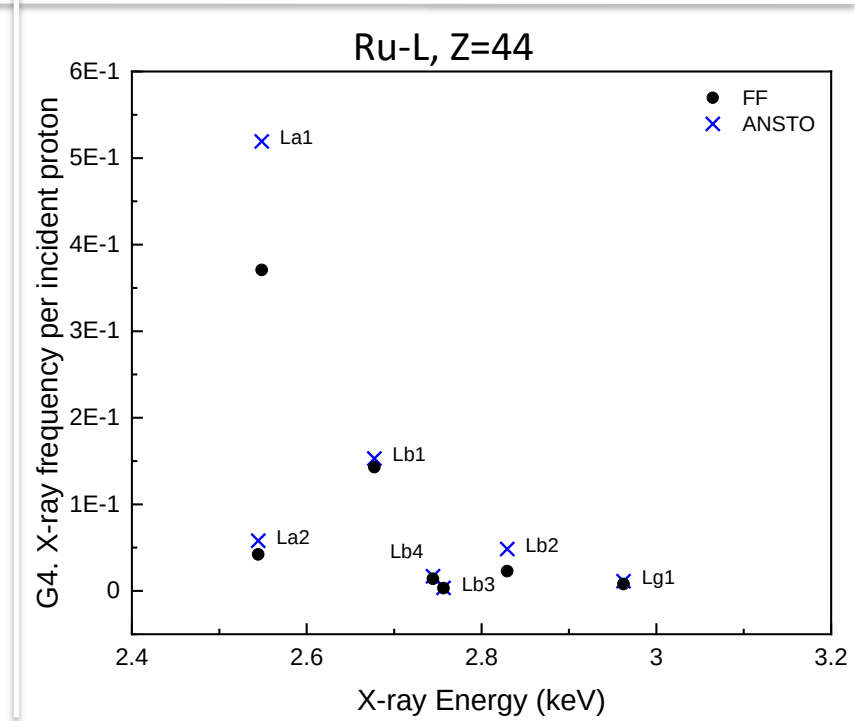

Ti-K, Z=22
FF
ANSTO
Exp. Frequency
Ka1
Ka2
G4. X-ray frequency per incident proton
X-ray Energy (keV)


Nb-K, Z=41
FF
ANSTO
Exp. Frequency
Ka1
Ka2
G4. X-ray frequency per incident proton
X-ray Energy (keV)

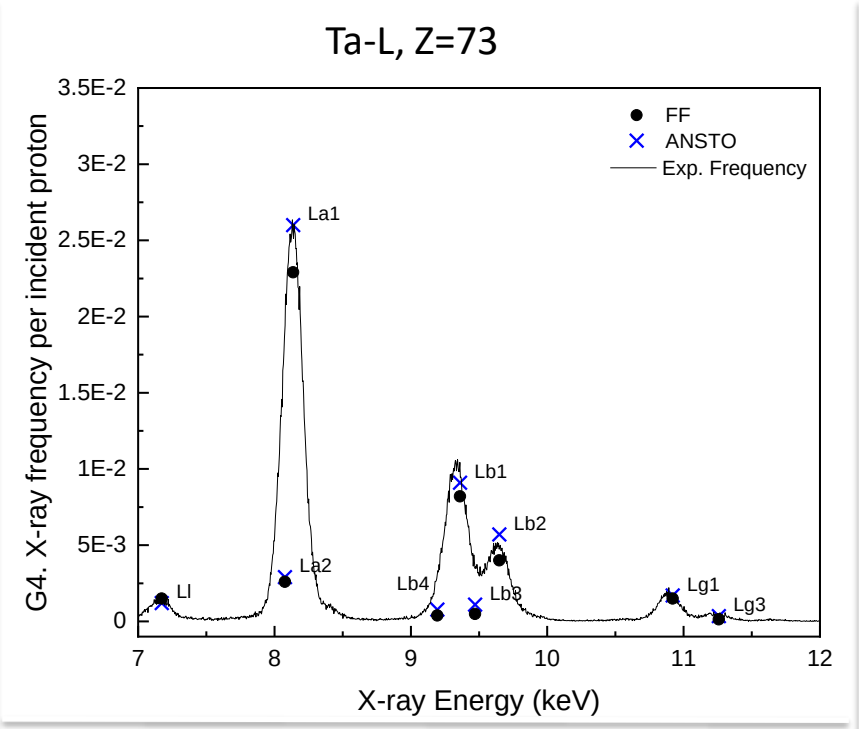

Ru-K, Z=44
FF
ANSTO
Exp. Frequency
Ka1
Ka2
G4. X-ray frequency per incident proton
X-ray Energy (keV)

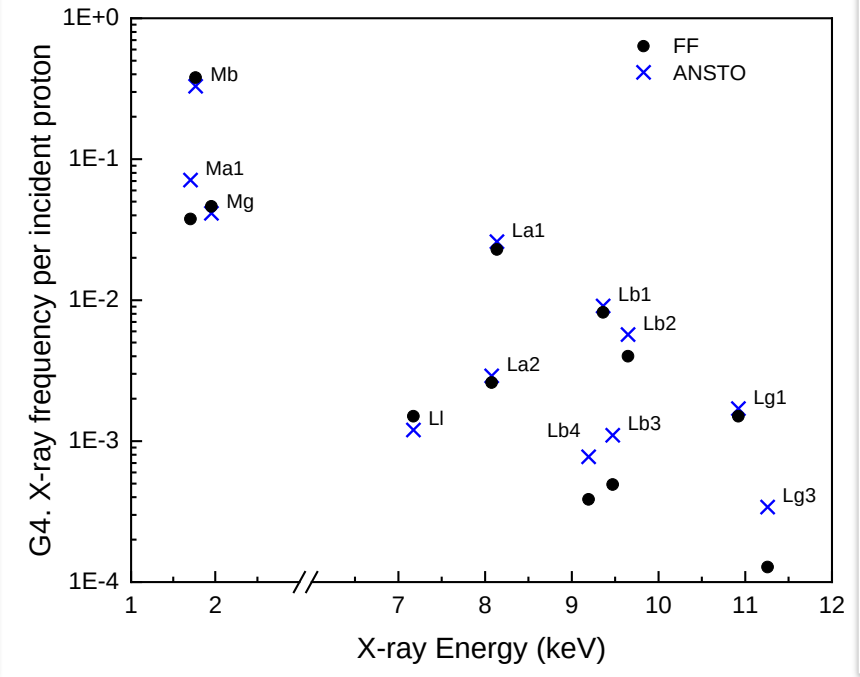

Zn-K, Z=30
FF
ANSTO
Exp. Frequency
Ka1
Ka2
G4. X-ray frequency per incident proton
X-ray Energy (keV)


Nb-L, Z=41
FF
ANSTO
La1
La2
Lb1
Lb2
Lb3
Lb4
Lg1
G4. X-ray frequency per incident proton
X-ray Energy (keV)


Ru-L, Z=44
FF
ANSTO
La1
La2
Lb1
Lb2
Lb3
Lb4
Lg1
G4. X-ray frequency per incident proton
X-ray Energy (keV)

10 MeV alpha


Ta-L, Z=73
G4. X-ray frequency per incident proton
X-ray Energy (keV)
FF
ANSTO
Exp. Frequency
La1
La2
Ll
Lb1
Lb2
Lb3
Lb4
Lg1
Lg3


G4. X-ray frequency per incident proton
X-ray Energy (keV)
FF
ANSTO
Mb
Ma1
Mg
La1
La2
Ll
Lb1
Lb2
Lb3
Lb4
Lg1
Lg3

Conclusion

- ANSTO library implemented in Geant4.
- emission X-ray spectra using the ANSTO approach provide similar or higher X-ray emission rates, depending on the energy of the incident particle and target material.
- ANSTO results show reasonable agreement with experimental data.
- The effect of the ANSTO library on the calculation of Auger yields need to be investigated.
- Once the ANSTO data libraries have been thoroughly investigated they will be released within the future Geant4 version.
- The PIXE proton and alpha cross sections will be released in 2021 (beta release of Geant4)