

# Geant4 X-ray fluorescence with ANSTO library

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

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 G4-ANSTO, modelling PIXE (p and  $\alpha$  ionisation cross sections and fluorescence yields) 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  $\alpha$  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.

*Nuclear Inst. and Methods in Physics Research B* 436 (2018) 285–291



## Latest Geant4 developments for PIXE applications

S. Bakr<sup>a,\*</sup>, D.D. Cohen<sup>b</sup>, R. Siegele<sup>b</sup>, S. Incerti<sup>c,d</sup>, V. Ivanchenko<sup>e,f</sup>, A. Mantero<sup>g</sup>, A. Rosenfeld<sup>a,h</sup>, S. Guatelli<sup>i,h</sup>



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

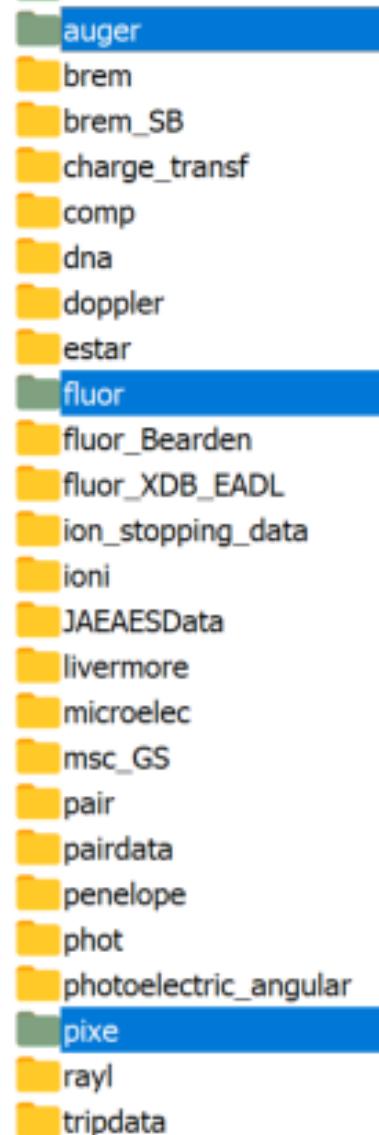
# PIXE in Geant4

## 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)** G4-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

## 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:
  - Based on Form Factor (Taborda K, L, M 2011-2013)
  - ANSTO PIXE cross section
- Transition probabilities:
  - EADL, G4EMLOW7.7
  - ANSTO-HF
    - 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/flu)
    - 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

	G4-default	G4-ANSTO
<b>Ionisation cross sections</b>	<i>ECPSSR Form Factor</i> [11], [12]	<i>ANSTO ECPSSR</i> [14]
<b>Transition probabilities</b>	<i>EADL</i> (Hartree-Slater) [19]	<i>ANSTO HF</i> (Hartree-Fock) [22]

## Track Your Accepted Article

The easiest way to check the publication status of your accepted article

### Geant4 X-ray fluorescence with updated libraries

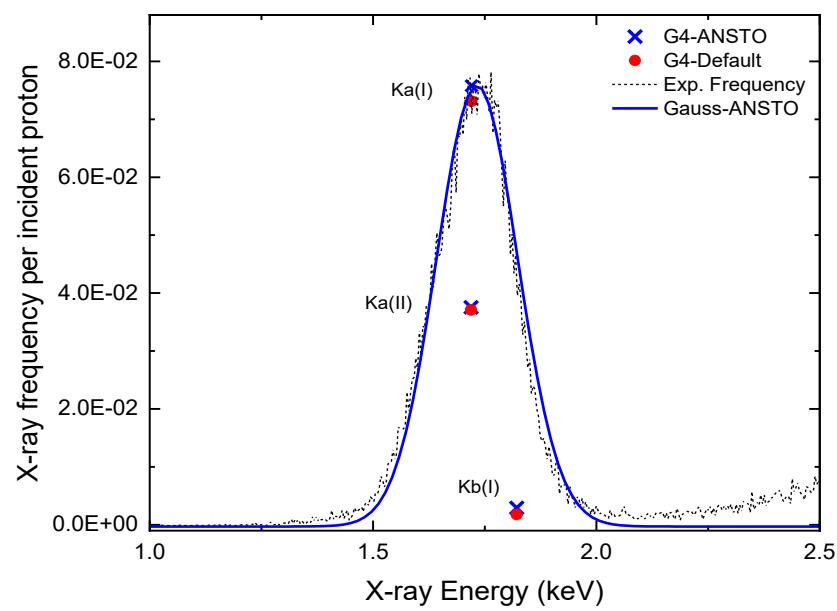
Article reference	NIMB64530
Journal	Nuclear Inst. and Methods in Physics Research, B
Corresponding author	Samer Bakr
First author	Samer Bakr
Received at Editorial Office	17 Jul 2021
Article revised	11 Sep 2021
Article accepted for publication	13 Sep 2021



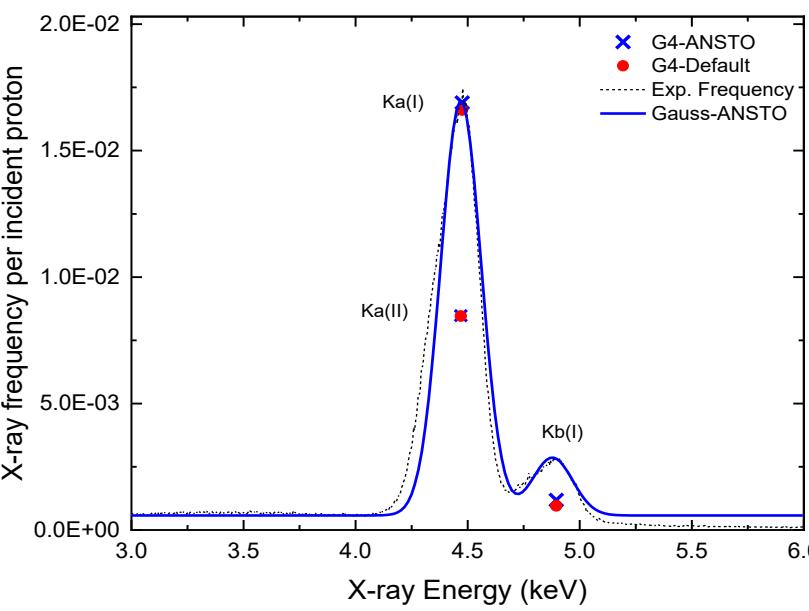
# Methodology

- **Geant4 TestEm5 extended example (Geant4 10.05.p01)**
  - Monochromatic beams of proton and alpha particles are incident on 25  $\mu\text{m}$  thick targets (50  $\mu\text{m}$  lateral sizes).
  - The new data library, G4-ANSTO, same format of the existing EADL Geant4 data library.
  - G4-ANSTO and EADL, has been quantified in terms of fluorescence X-ray yields per incident particle.

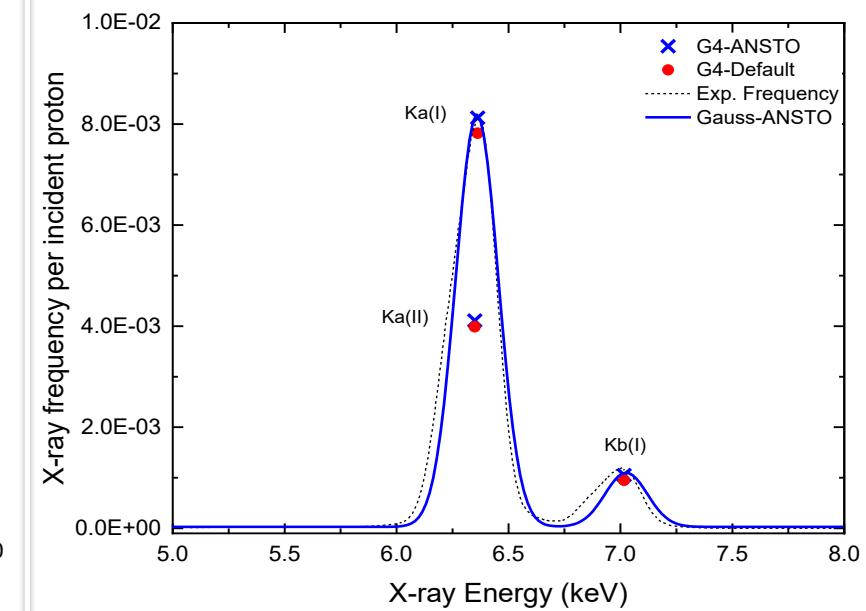
2 MeV proton Si-K, Z=14



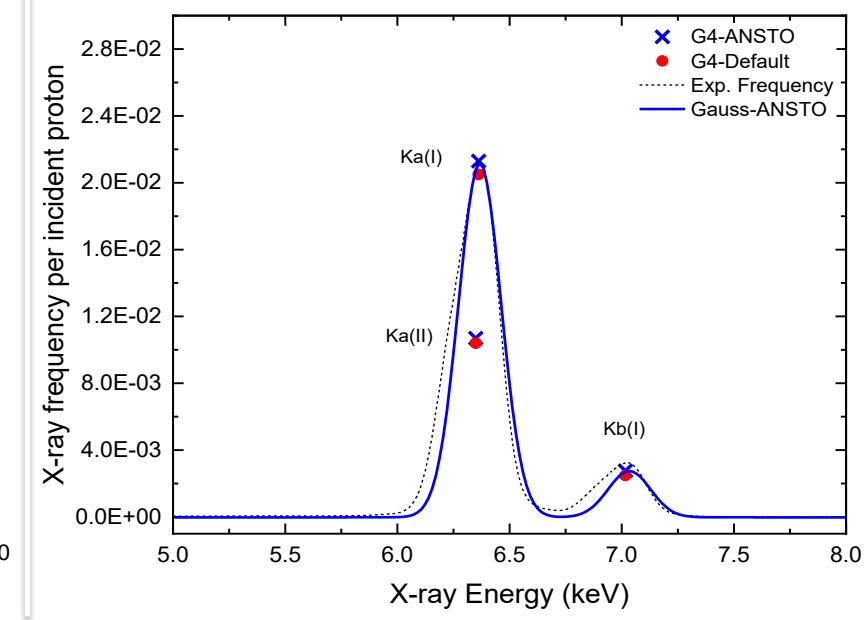
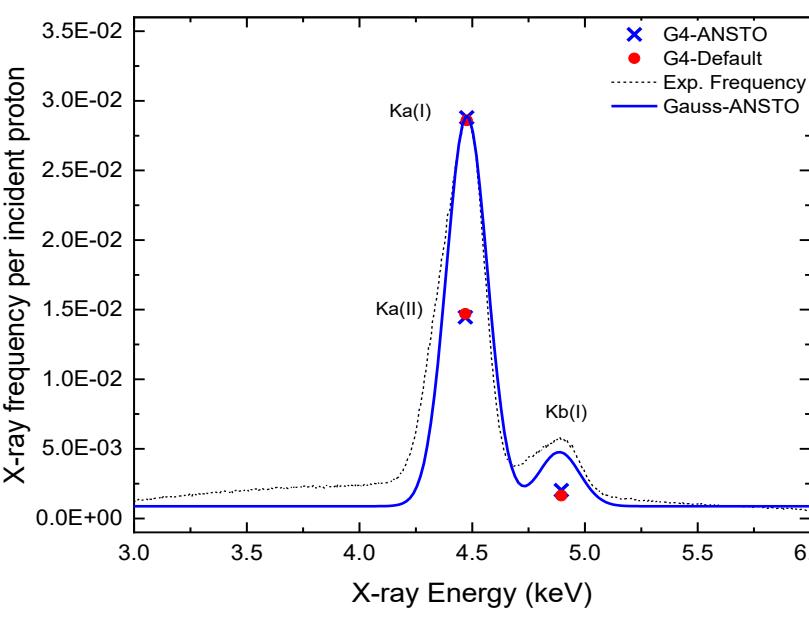
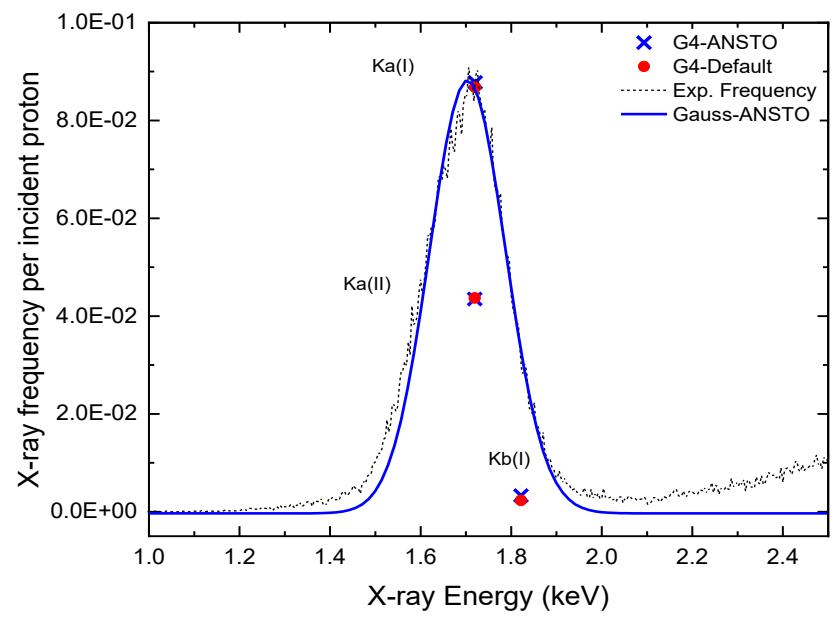
Ti-K, Z=22



Fe-K, Z=26

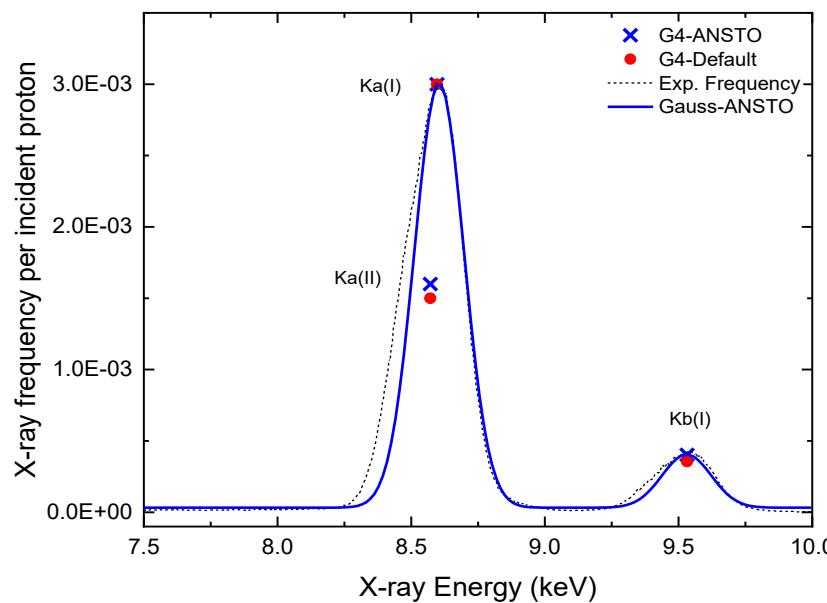


3 MeV proton

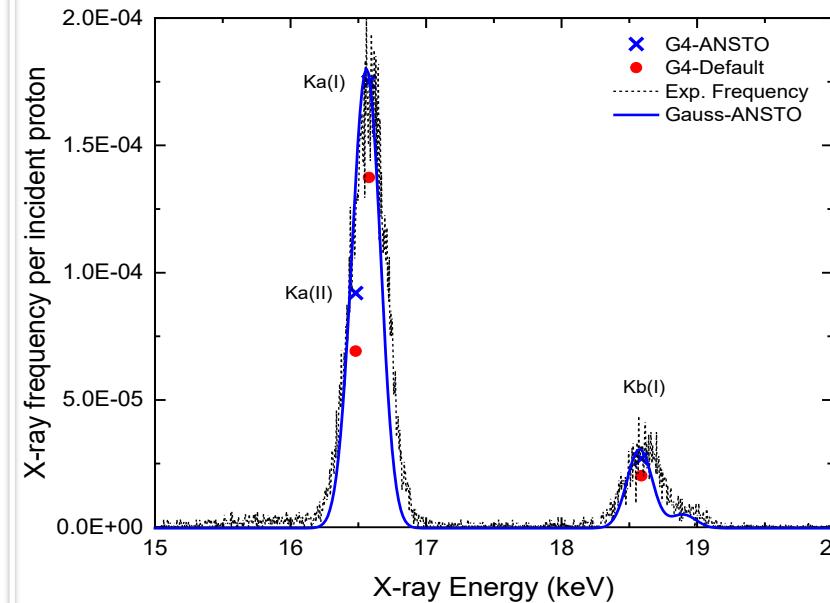


2 MeV proton

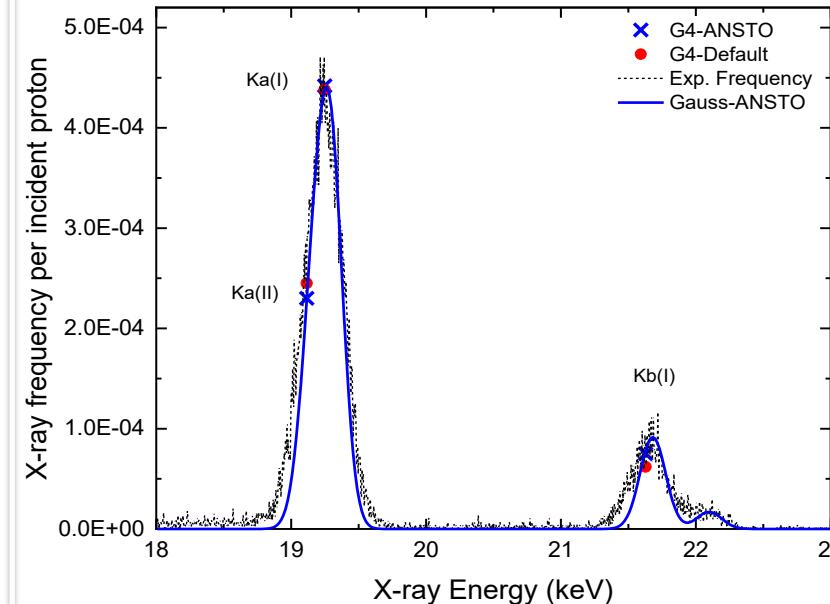
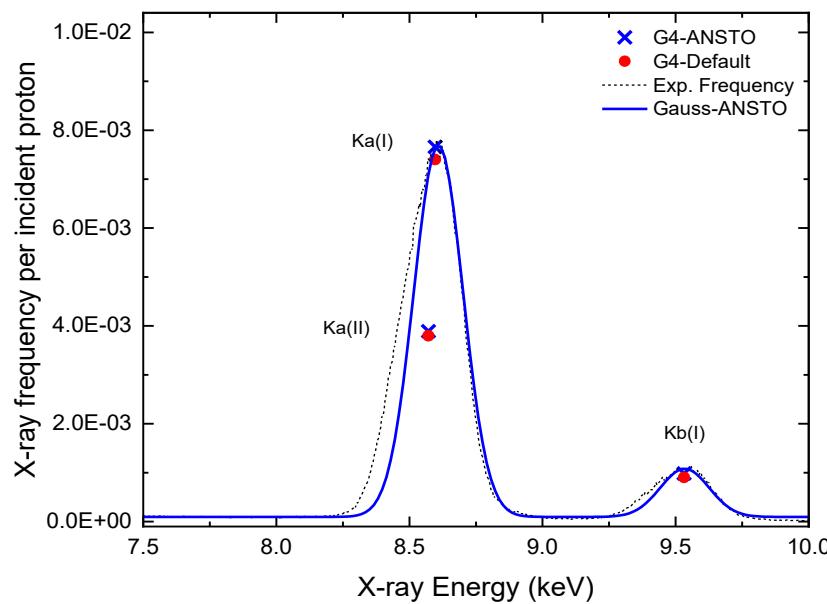
Zn-K, Z=30



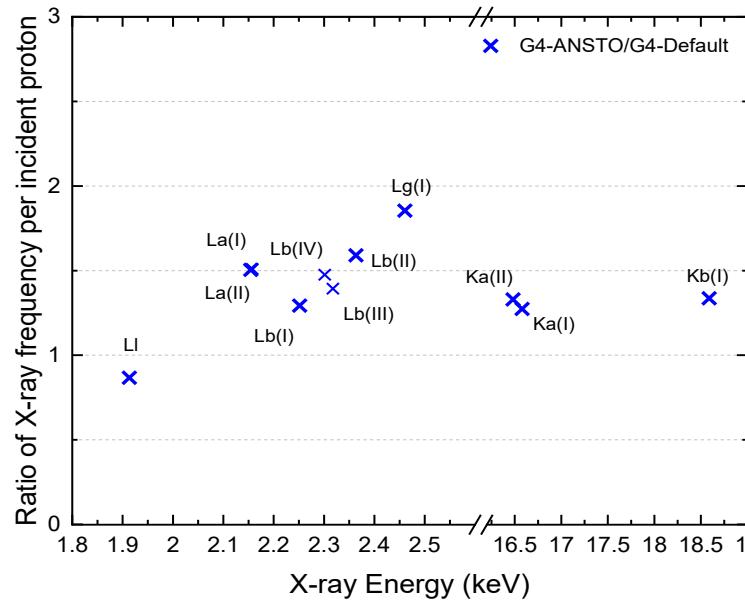
Nb-K, Z=41



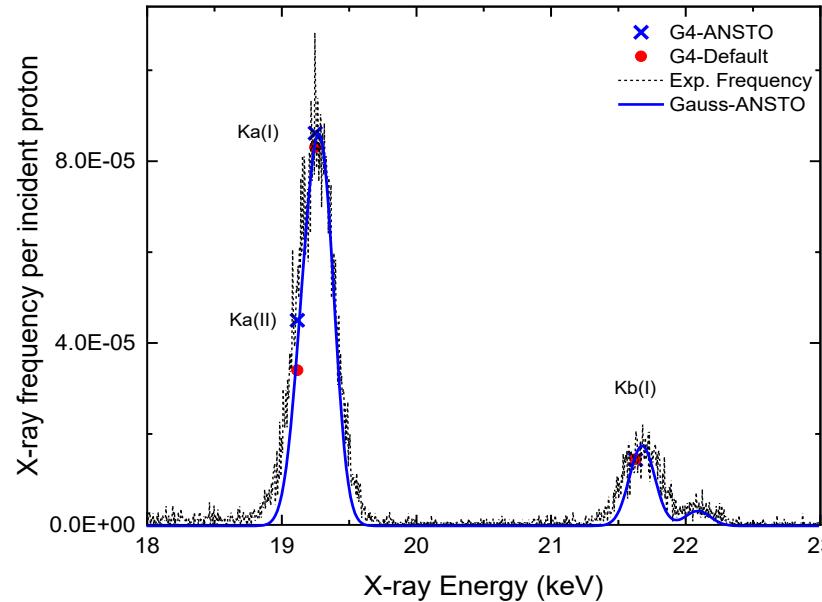
3 MeV proton



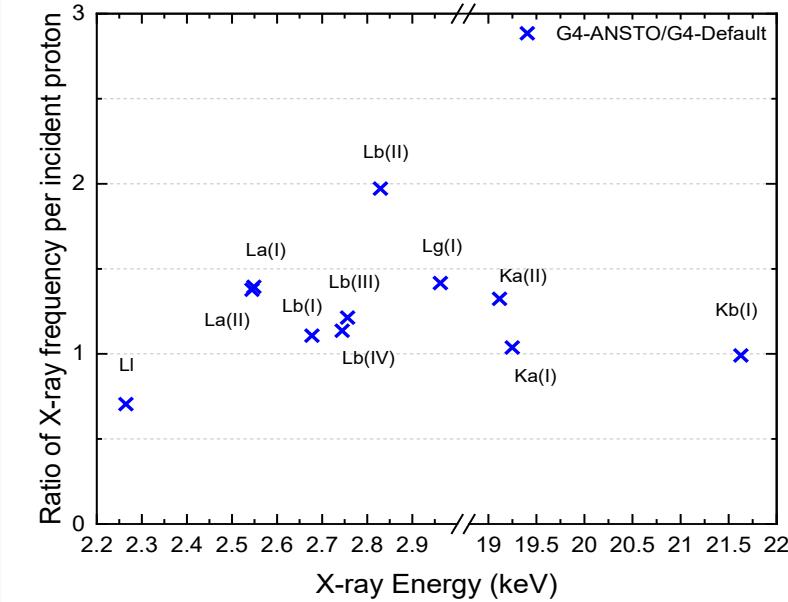
2 MeV proton Nb-L, Z=41



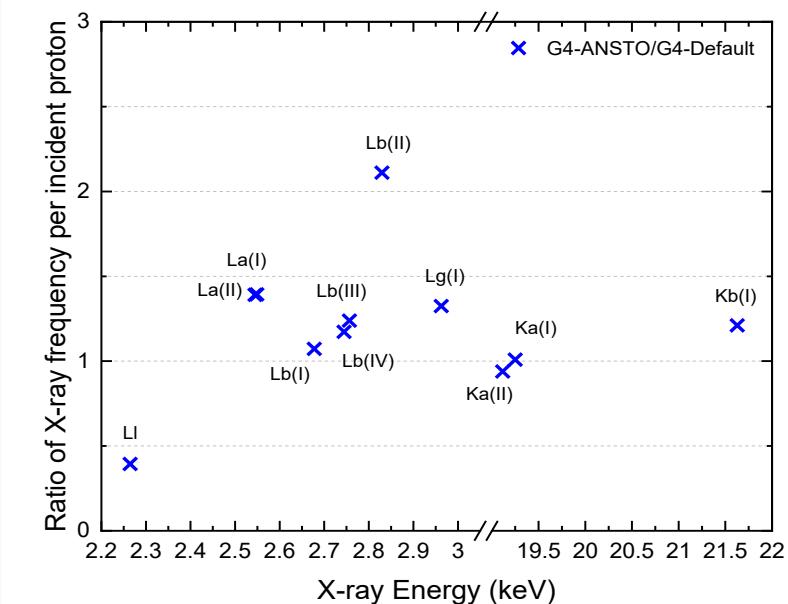
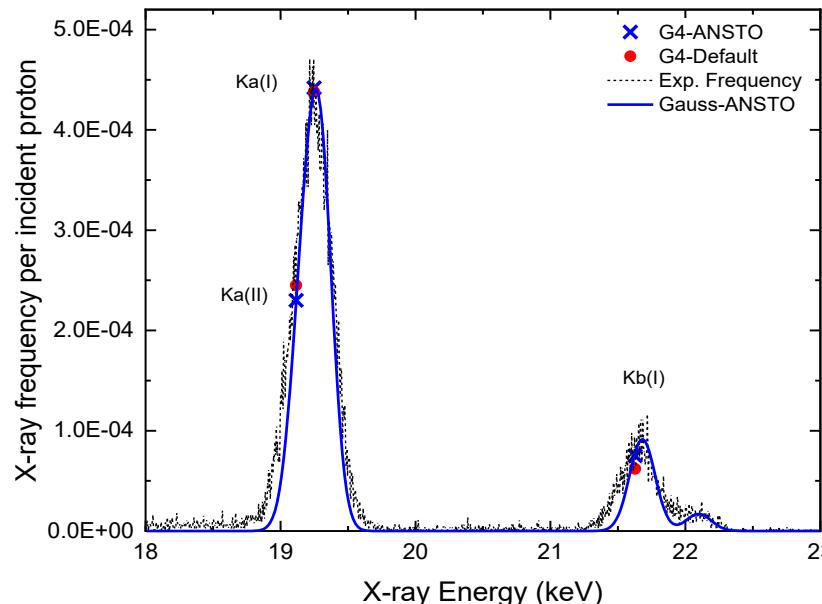
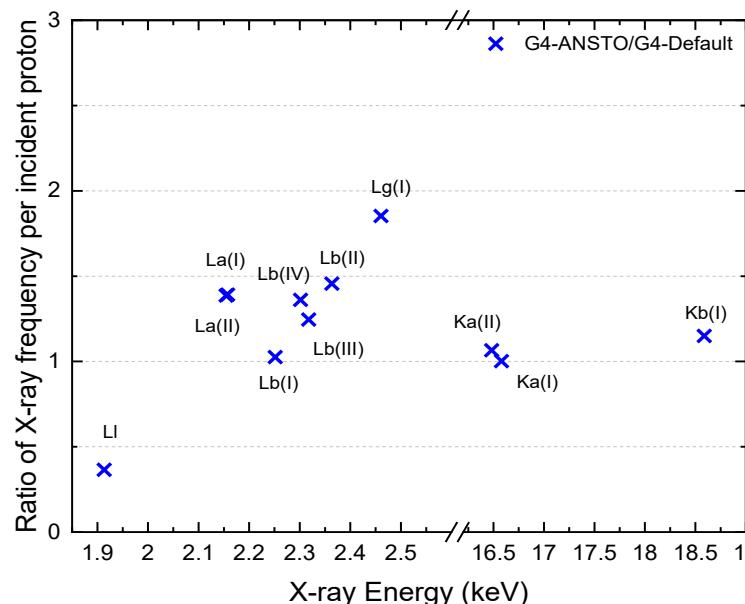
Ru-K, Z=44



Ru-L, Z=44

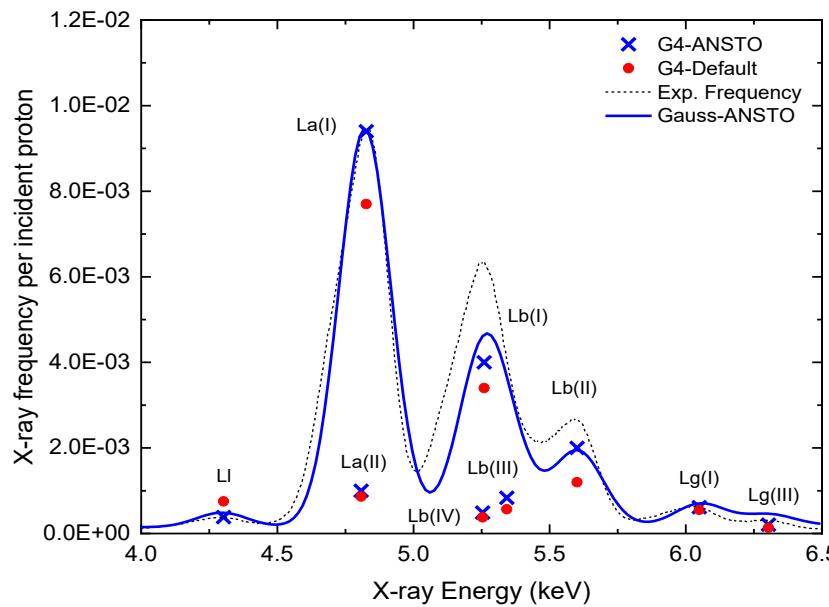


3 MeV proton

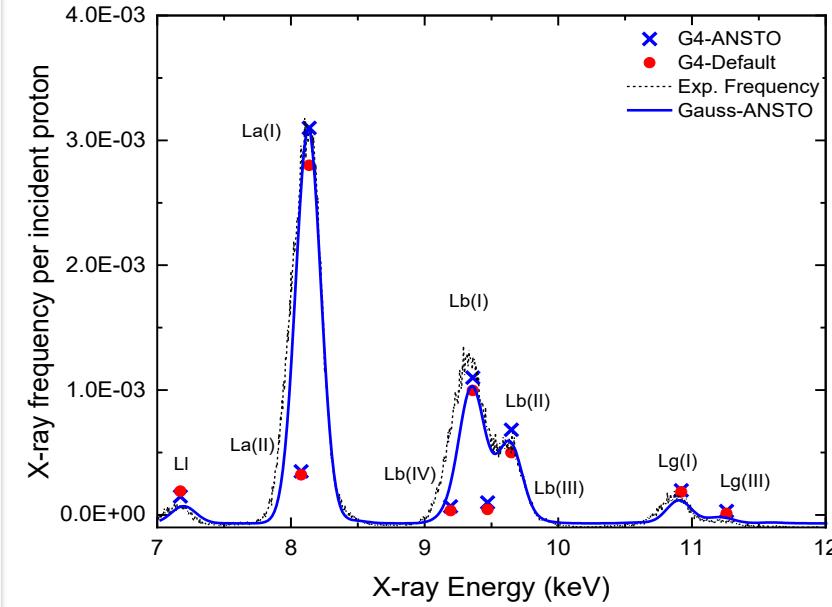


2 MeV proton

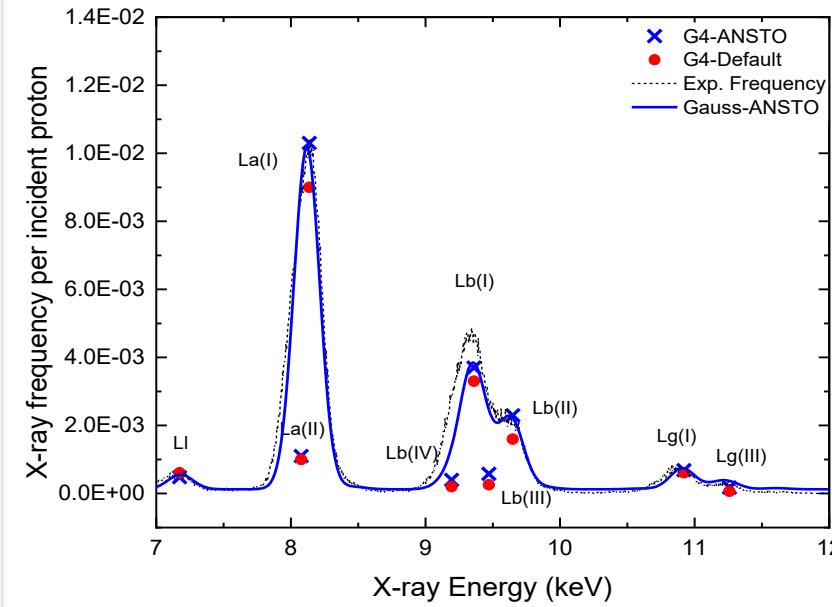
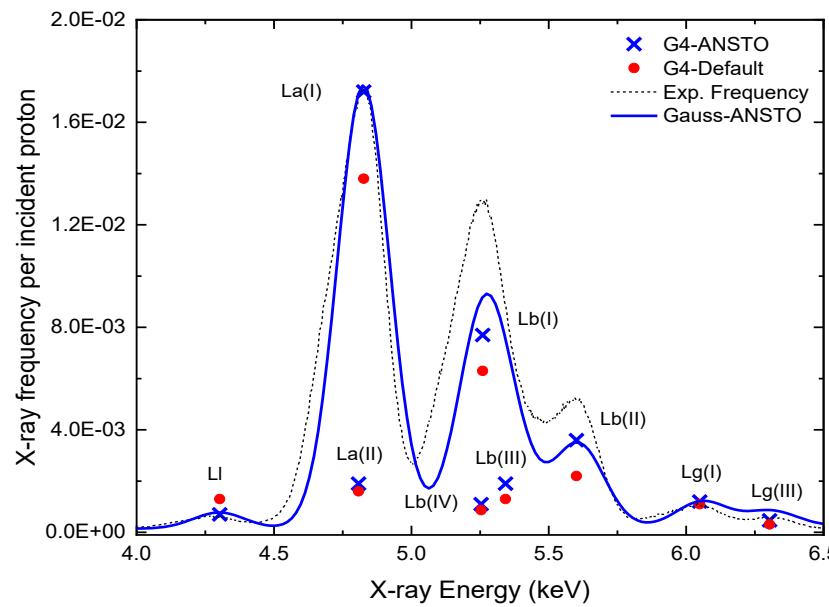
Ce-L, Z=58



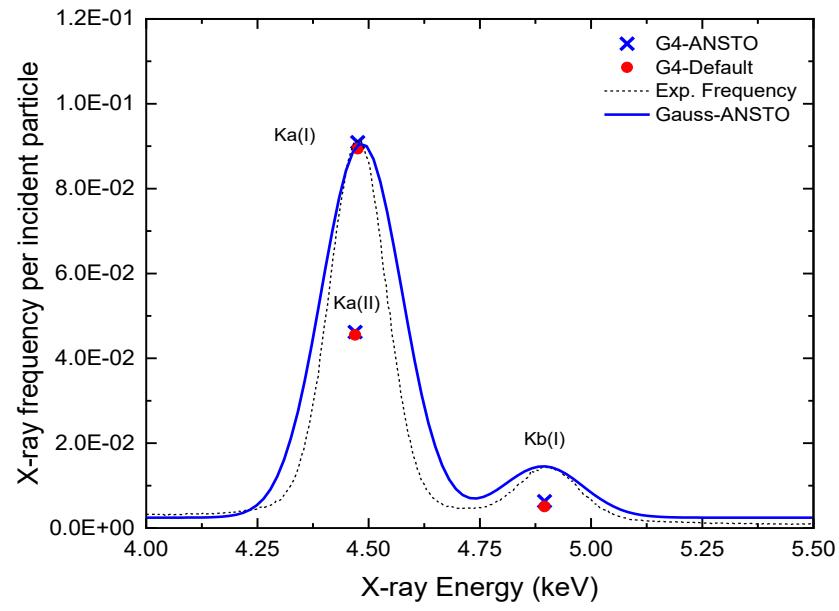
Ta-L, Z=73



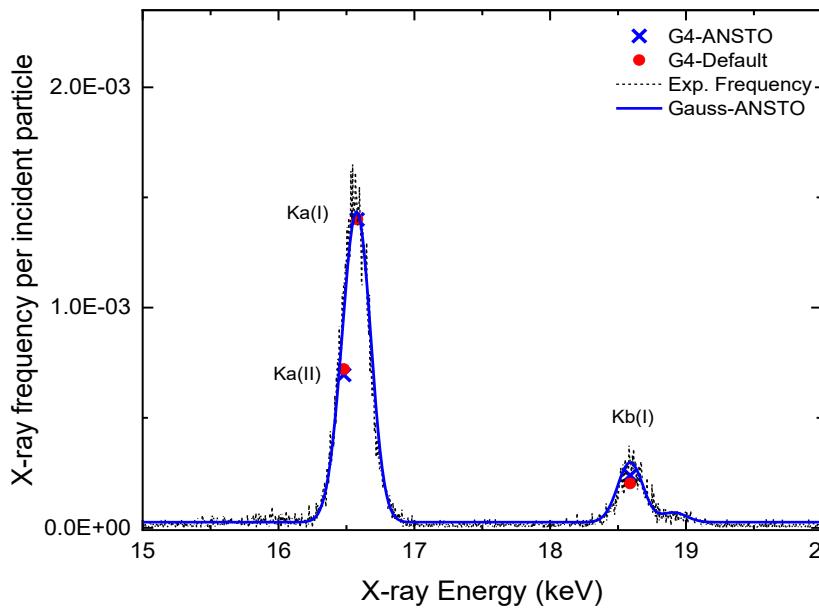
3 MeV proton



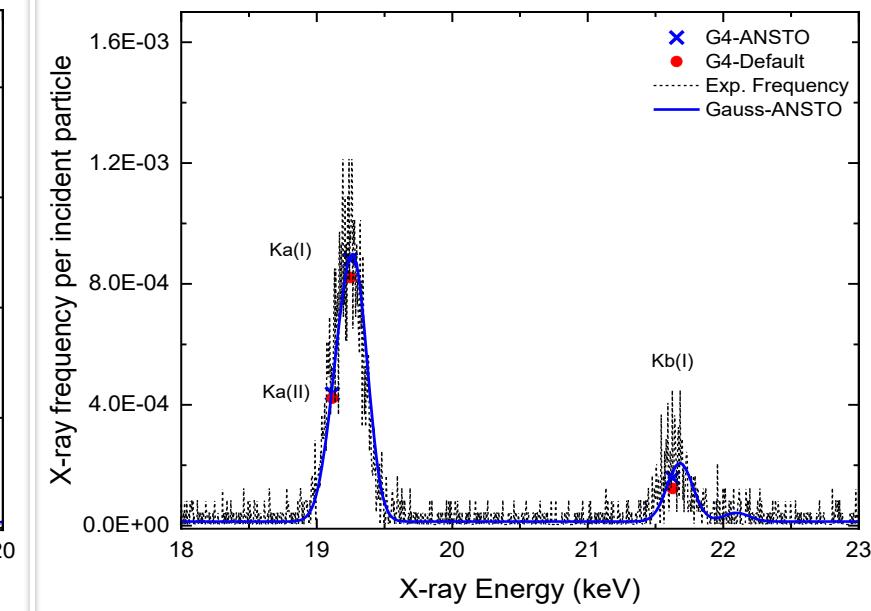
10 MeV alpha Ti-K, Z=22



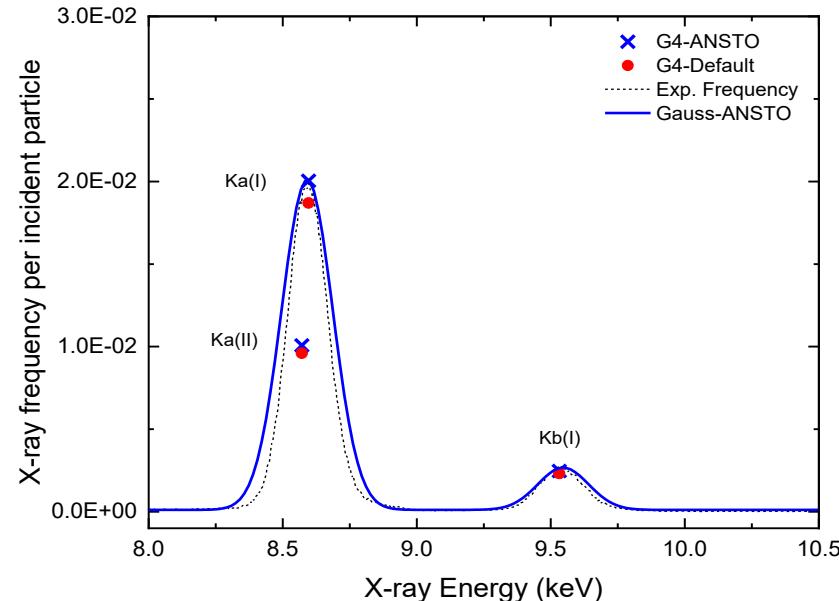
Nb-K, Z=41



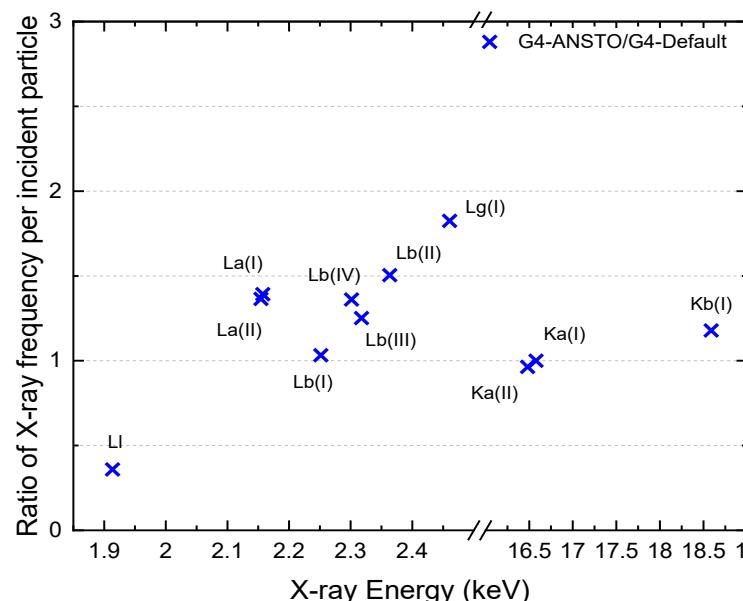
Ru-K, Z=44



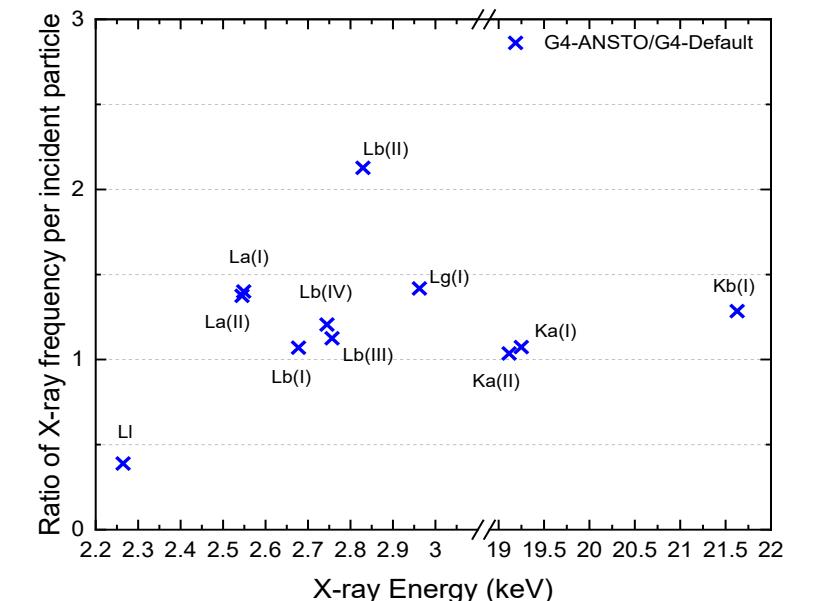
Zn-K, Z=30



Nb-L, Z=41

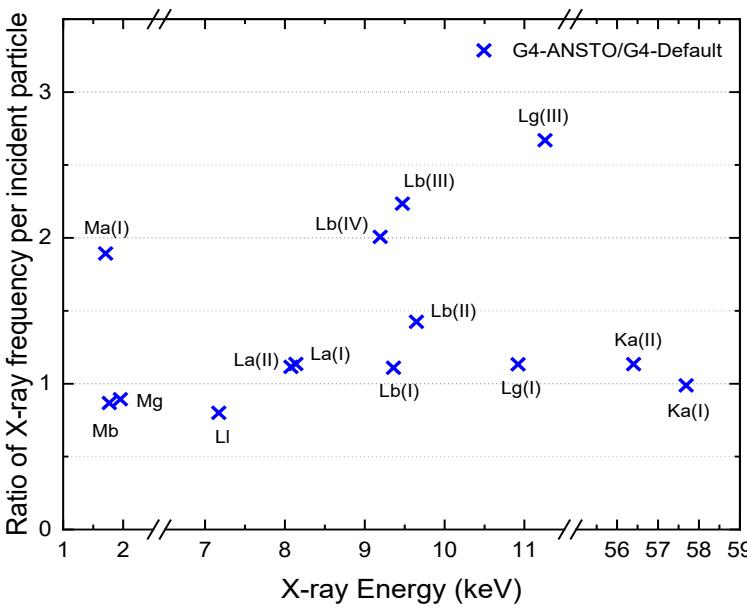
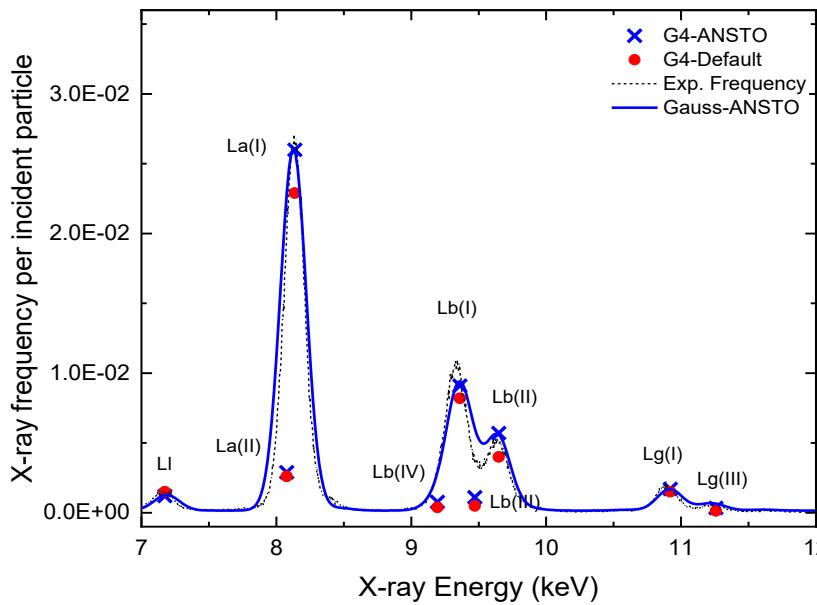


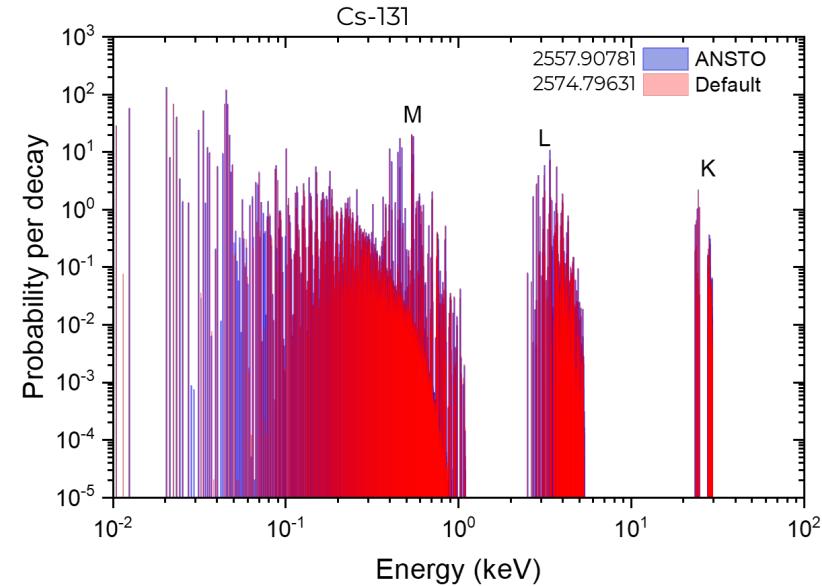
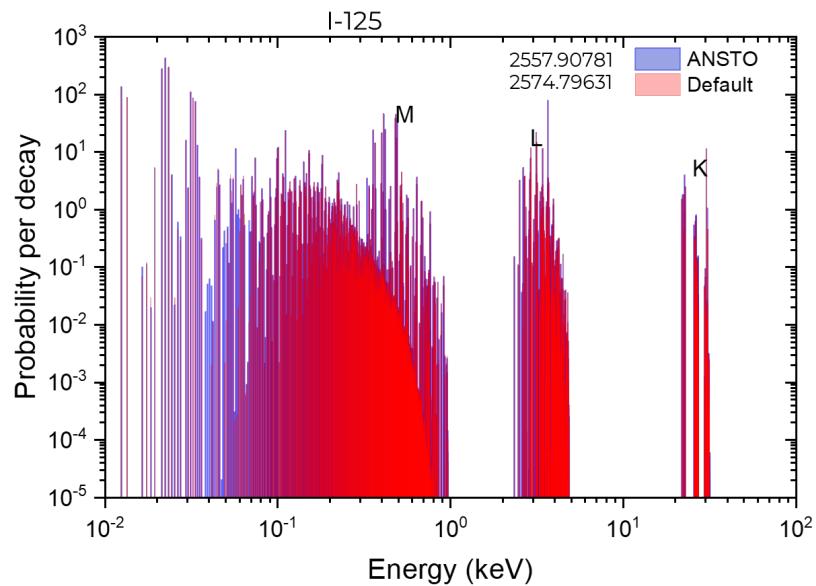
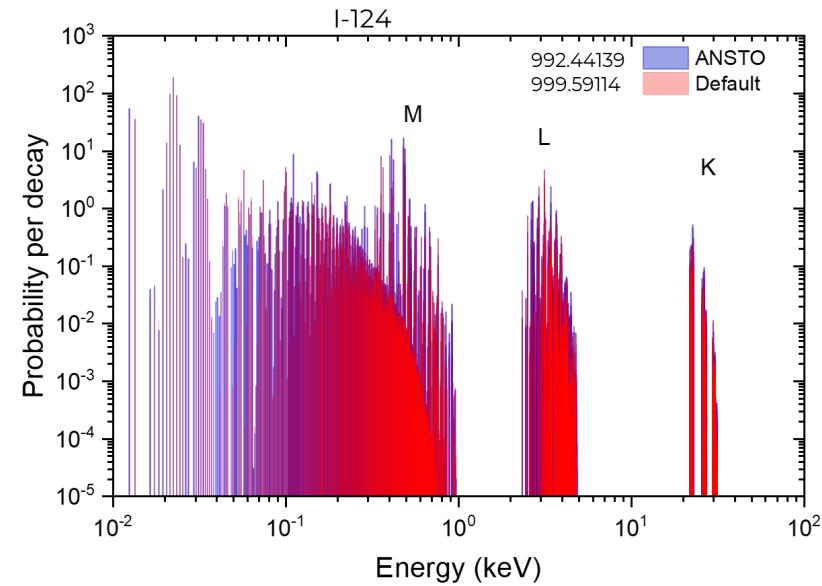
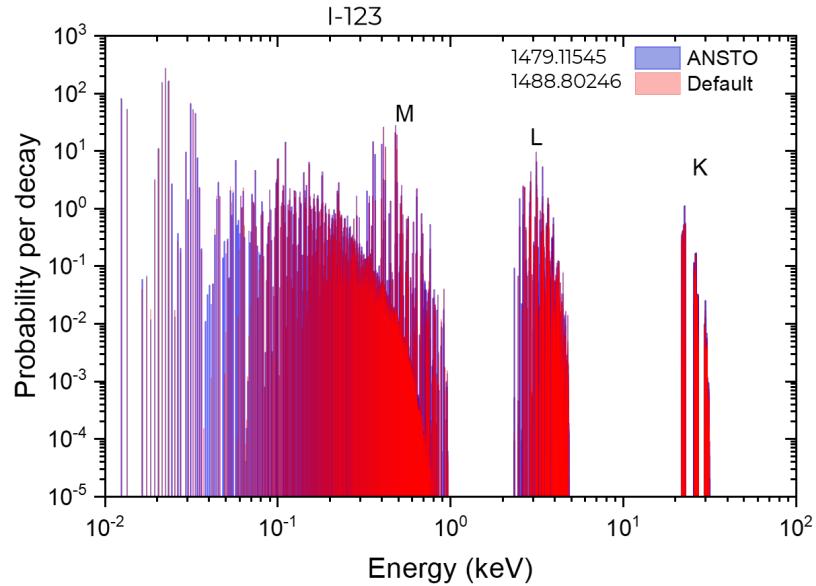
Ru-L, Z=44

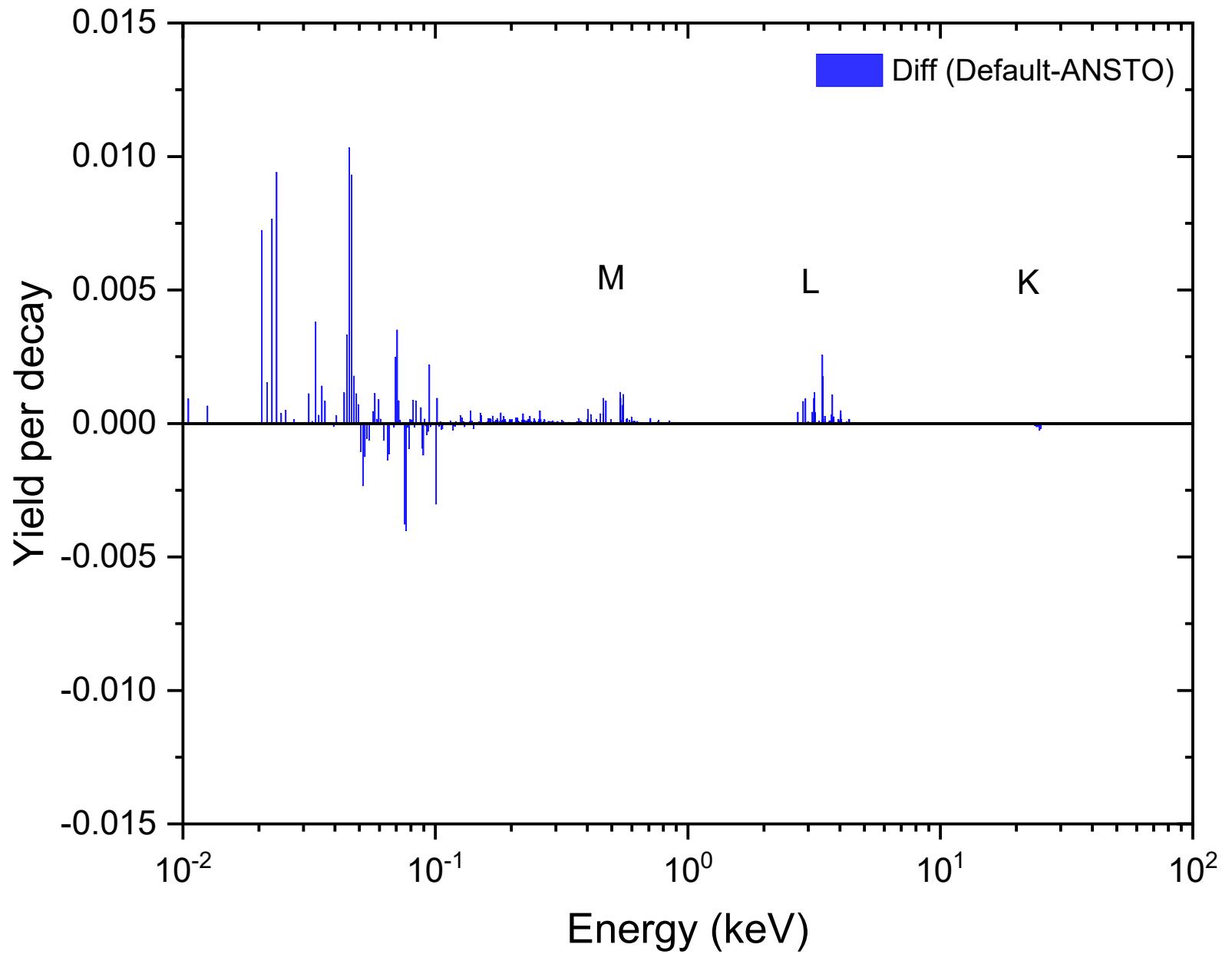


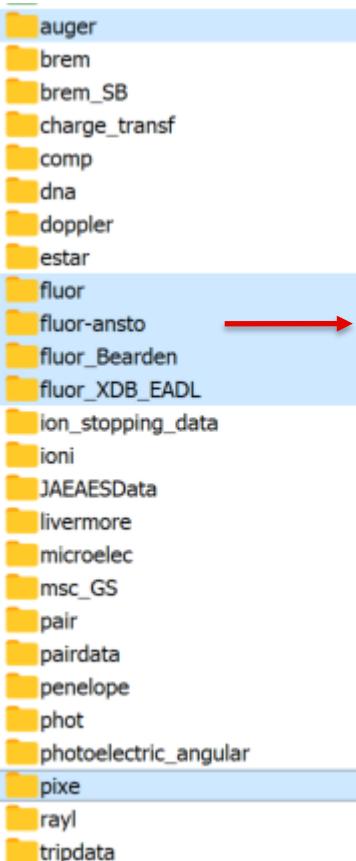
10 MeV alpha

### Ta-L, Z=73









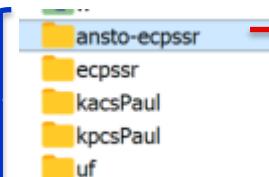
## Track Your Accepted Article

The easiest way to check the publication status of your accepted article

### Geant4 X-ray fluorescence with updated libraries

Article reference	NIMB64530
Journal	Nuclear Inst. and Methods in Physics Research, B
Corresponding author	Samer Bakr
First author	Samer Bakr
Received at Editorial Office	17 Jul 2021
Article revised	11 Sep 2021
Article accepted for publication	13 Sep 2021

ANSTO HF

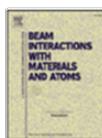


Nuclear Inst. and Methods in Physics Research B 436 (2018) 285-291

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research B

journal homepage: [www.elsevier.com/locate/nimb](http://www.elsevier.com/locate/nimb)



### Latest Geant4 developments for PIXE applications

S. Bakr<sup>a,c</sup>, D.D. Cohen<sup>b</sup>, R. Siegele<sup>b</sup>, S. Incerti<sup>c,d</sup>, V. Ivanchenko<sup>e,f</sup>, A. Mantero<sup>e</sup>, A. Rosenfeld<sup>a,h</sup>, S. Guatelli<sup>a,h</sup>

<sup>a</sup>CMRR, University of Wollongong, Australia

<sup>b</sup>Centre for Accelerator Science, Australian Nuclear Science and Technology Organization, Australia

<sup>c</sup>CNRS-IN2P3, Centre d'Etudes Nucléaires de Bordeaux-Codognan, France

<sup>d</sup>Université de Bordeaux, Centre d'Etudes Nucléaires de Bordeaux-Codognan, France

<sup>e</sup>Geant4 Associates International Ltd, United Kingdom

<sup>f</sup>Tomsk State University, Russia

<sup>g</sup>SWIARD srl, Italy

<sup>h</sup>Illawarra Health and Medical Research Institute, University of Wollongong, NSW, Australia



## geant4/source/processes/electromagnetic/lowenergy/src/

G4ANSTOFormFactorKxsModel.cc  
G4ANSTOFormFactorLixsModel.cc  
G4ANSTOFormFactorMixsModel.cc

```
G4ANSTOecpssrLixsModel::G4ANSTOecpssrLixsModel()
{
    G4cout << "Using ANSTO L Cross Sections! " << G4endl;
    interpolation = new G4LinInterpolation();

    for (G4int i=26; i<93; i++)
    {
        protonL1DataSetMap[i] = new G4EMDataSet(i,interpolation);
        protonL1DataSetMap[i]->LoadData("pixe/ansto/proton/l1-");

        protonL2DataSetMap[i] = new G4EMDataSet(i,interpolation);
        protonL2DataSetMap[i]->LoadData("pixe/ansto/proton/l2-");

        protonL3DataSetMap[i] = new G4EMDataSet(i,interpolation);
        protonL3DataSetMap[i]->LoadData("pixe/ansto/proton/l3-");
    }

    for (G4int i=26; i<93; i++)
    {
        alphaL1DataSetMap[i] = new G4EMDataSet(i,interpolation);
        alphaL1DataSetMap[i]->LoadData("pixe/ansto/alpha/l1-");

        alphaL2DataSetMap[i] = new G4EMDataSet(i,interpolation);
        alphaL2DataSetMap[i]->LoadData("pixe/ansto/alpha/l2-");

        alphaL3DataSetMap[i] = new G4EMDataSet(i,interpolation);
        alphaL3DataSetMap[i]->LoadData("pixe/ansto/alpha/l3-");
    }
}
```

geant4/source/processes/electromagnetic/lowenergy/src/

G4teoCrossSection.cc

```
G4teoCrossSection::G4teoCrossSection(const G4String& nam)
  :G4VhShellCrossSection(nam), totalCS(0.0)
{
  ecpssrShellMi = nullptr;
  if (nam == "ECPSSR_Analytical")
  {
    ecpssrShellK  = new G4ecpssrBaseKxsModel();
    ecpssrShellLi = new G4ecpssrBaseLixsModel();
  }
  else if (nam == "ECPSSR_FormFactor")
  {
    ecpssrShellK  = new G4ecpssrFormFactorKxsModel();
    ecpssrShellLi = new G4ecpssrFormFactorLixsModel();
    ecpssrShellMi = new G4ecpssrFormFactorMixsModel();
  }
  | else if (nam == "ECPSSR_ANSTO")
  {
    ecpssrShellK  = new G4ANST0ecpssrKxsModel();
    ecpssrShellLi = new G4ANST0ecpssrLixsModel();
    ecpssrShellMi = new G4ANST0ecpssrMixsModel();
  }
  else
  {
    G4cout << "G4teoCrossSection::G4teoCrossSection: ERROR "
      << " in cross section name ECPSSR_Analytical is used"
      << G4endl;
    ecpssrShellK  = new G4ecpssrBaseKxsModel();
    ecpssrShellLi = new G4ecpssrBaseLixsModel();
  }
}
```

geant4/source/processes/electromagnetic/lowenergy/src/

G4UAtomicDeexcitation.cc

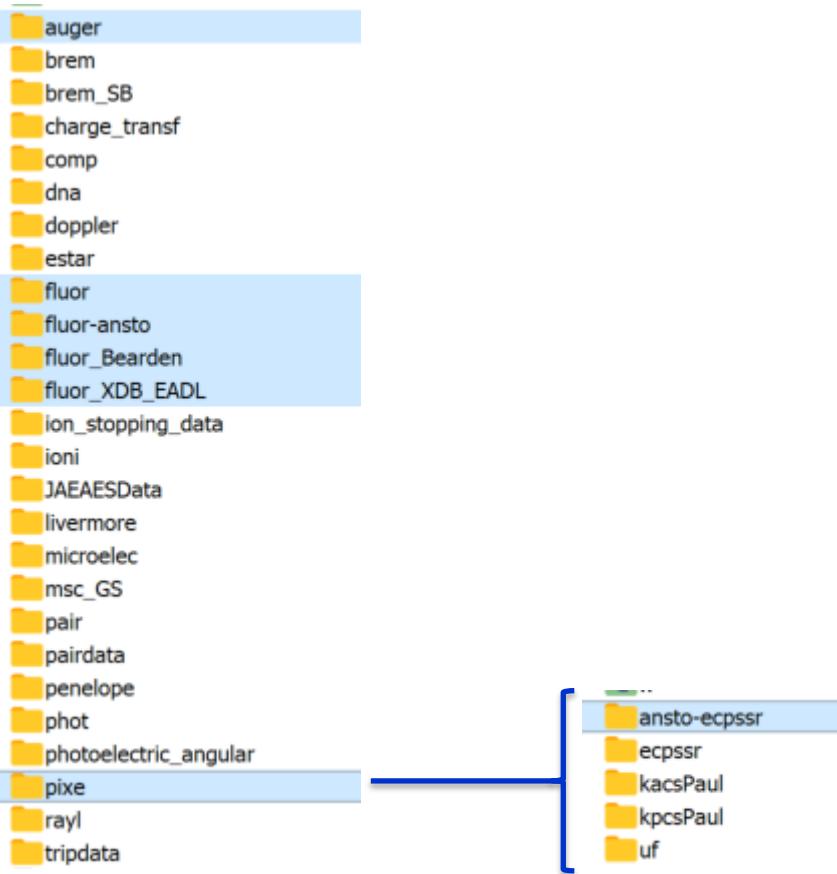
```
// Instantiate new proton/ion cross section
if(!PIXEshellCS) {
    if (namePIXExsModel == "ECPSSR_FormFactor")
    {
        PIXEshellCS = new G4teoCrossSection(namePIXExsModel);
    }

    else if(namePIXExsModel == "ECPSSR_ANSTO")
    {
        PIXEshellCS = new G4teoCrossSection(namePIXExsModel);
    }

    else if(namePIXExsModel == "Empirical")
    {
        PIXEshellCS = new G4empCrossSection(namePIXExsModel);
    }
}

//G4cout << "PIXE is initialised" << G4endl;
```

/geant4.10.05.p01-build/data/G4EMLOW7.7/



Part of the user macro

```
/process/em/deexcitationIgnoreCut true  
#/process/em/deexcitation world true false true  
/process/em/fluo true  
/process/em/pixe true  
/process/em/auger true  
  
#/process/em/pixeXSmodel ECPSSR_FormFactor  
/process/em/pixeXSmodel ECPSSR_ANSTD  
#/process/em/pixeXSmodel ECPSSR_Analytical  
#/process/em/pixeXSmodel Empirical  
  
/process/em/augerCascade true  
/process/em/lowestElectronEnergy 10 eV  
  
/run/initialize
```

# 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.
- Geant4 ANSTO approach results show reasonable agreement with experimental data.
- The effect of the ANSTO library on the calculation of Auger yields has been investigated.
- We suggest the ANSTO data libraries (ICS and fluo) to be released within the future Geant4 version.