# ***MottCalc***

*Mott Calculator, a new tool for calculating elastic Mott scattering differential cross sections for analytical purposes*

*User Guide*

# Introduction

The present work aims at introducing the features and functionalities of the MottCalc Excel Spreadsheet and MottCalc application as well as presenting the theoretical background behind their creation. MottCalc is an analytical code developed for the theoretical calculation of differential cross section distributions (angular or energy) of Mott scattering.

The text is divided into three chapters. Chapter one contains a brief overview of the general case of elastic scattering as well as the theoretical aspects of Mott scattering and how it differs from the general (standard) Rutherford case. The expressions found in this chapter were implemented in the program. The second chapter is devoted to the installation and use of the Excel spreadsheet, while the third chapter describes the installation process and functionality of the stand-alone application.

# 1. Physics

## 1.1 Elastic Scattering

In the general case of elastic scattering where the mass of the incident nucleus ($M_1$) is less or equal than the mass of the target nucleus ($M_2$), the relation between the kinetic energies of the scattered and recoil nuclei is given by the expression [Mayer_77]

$$E_{recoil,lab} = E_{0,lab} - E_{scattered,lab} \quad (1)$$

where $E_{recoil,lab}$ and $E_{scattered,lab}$ refer to the kinetic energy of the recoil and scattered nucleus in the Lab frame of reference while $E_0$ is the initial kinetic energy of the projectile. $E_{scattered,lab}$ is given by the expression [Mayer_77]

$$E_{scattered,lab} = E_{0,lab} \frac{\{x\cos(\theta_{lab}) + [1 - x^2 \sin^2(\theta_{lab})]^{1/2}\}^2}{(1+x)^2} \quad (2)$$

where $x$ stands for the mass ratio $\frac{M_1}{M_2}$. Accordingly, the relation between the laboratory detection angles of the nuclei is given by [Mayer_77]:

$$\theta = \pi - 2\phi_{lab} \quad (3)$$

where $\theta_{lab}$ is the laboratory detection angle of the scattered nucleus and $\phi_{lab}$ the laboratory angle of the recoil nucleus. $\theta$ and $\phi$ refer to the respective angles in the center of mass frame of reference. $\theta$ is equal to [Mayer_77]:

$$\theta = \theta_{lab} + \sin^{-1}[x\sin(\theta_{lab})] \quad (4)$$

Finally, the relation between the differential cross sections in the lab and center of mass reference frames is given by the following expression [Mayer_77]

$$\sigma(\theta)_{lab} = \sigma(\theta)_{cm} \frac{d\Omega_{cm}}{d\Omega_{lab}} \quad (5)$$

where (using classical reaction kinematics):

$$\frac{d\Omega_{cm}}{d\Omega_{lab}} = \frac{(1 + 2\gamma\cos\theta + \gamma^2)^{3/2}}{|1 + \gamma\cos\theta|} \quad (6a)$$

where $\gamma$ is equal to the ratio $\frac{v_{cm}}{v_{scattered}}$. The velocity $v_{cm}$ refers to the velocity of the *center of mass* system as measured in the lab reference frame. [Mayer_77]. $\gamma$, for a generic nuclear reaction of the type a+X--->b+Y, can also be expressed as follows:

$$\gamma = \left[ \frac{m_a m_b}{m_X m_Y} \frac{K_a}{K_a + Q\left(1 + m_a / m_X\right)} \right]^{1/2} \quad (6b)$$

## 1.2 Mott Scattering

Mott scattering refers to the elastic scattering of identical nuclei. For Mott scattering the mass ratio (x) is equal to 1 and Q=0, which leads to the following simplified results

$$\theta = 2\theta_{lab} \tag{7}$$

$$\theta_{lab} = \frac{\pi}{2} - \phi_{lab} \tag{8}$$

$$E_{scattered} = E_0\, cos^2(\theta_{lab}) \tag{9}$$

$$E_{recoil} = E_0\, sin^2(\theta_{lab}) = E_0\, cos^2(\varphi_{lab}) \tag{10}$$

$$\gamma = 1 \tag{11}$$

$$\frac{d\Omega_{cm}}{d\Omega_{lab}} = 2^{3/2}\sqrt{1+\cos\theta} \tag{12}$$

In any experimental setup, a detector will record both the scattered and recoil nuclei. Its position determines the detection angle which will be the same for both nuclei. For $\theta_{lab} = \phi_{lab}$ in Mott scattering both scattered and recoil nuclei have the same kinetic energy as shown in expressions (9) and (10). Since the nuclei are identical, there is no process of separating and distinguishing between the two, resulting in the creation of a single energy peak where both nuclei contribute. The resulting differential cross section would be expected to be equal to:

$$\frac{d\sigma_{total}}{d\Omega} = f^2_{scattered} + f^2_{recoil} \tag{13}$$

However due to the indistinguishability principle the addition of these two cross sections must be done quantum mechanically. This results in the appearance of an interference term in the total cross section. [Canto_14]

$$\frac{d\sigma_{total}}{d\Omega} = (f_{scattered} \pm f_{recoil})^2 \tag{14}$$

$$\frac{d\sigma_{total}}{d\Omega} = |f|^2_{scattered} + |f|^2_{recoil} \pm 2R|f|_{scattered}|f|_{recoil} \tag{15}$$

where $f$ refers to the scattering amplitudes. The sign depends on whether the nuclei are bosons or fermions due to the required symmetry or anti-symmetry of their wave function respectively. In the case of spin multiplicity (spin $\neq 0$ ) the cross section of each nucleus is an incoherent sum of the various possible total spin states. The final total differential cross section is a symmetrical or anti-symmetrical incoherent sum of the various cross sections of the scattered and recoil nuclei along with their signs and weighing factors that are determined by the spin multiplicity. This type of scattering was first studied by Mott in the 30's who calculated the analytical formula that determines the cross section for this type of scattering. For nuclei with spin *s*, atomic number *Z*, initial beam energy *E* and detection angle $\theta$, the Mott differential cross section in the center of mass reference frame is given by the expression (which combines bosons and fermions) [Canto_14]:

$$\frac{d\sigma}{d\Omega} = \left(\frac{1}{4\pi\varepsilon_0}\frac{Z^2e^2}{4E}\right)^2\left\{\frac{1}{sin^4(\frac{\theta}{2})} + \frac{1}{cos^4(\frac{\theta}{2})} + \frac{2(-1)^{2s}}{2s+1}\frac{\cos[n_s\ln(tan^2(\frac{\theta}{2}))]}{sin^2(\frac{\theta}{2})cos^2(\frac{\theta}{2})}\right\} \quad (16)$$

The first term of the formula corresponds to the scattered projectile, the second to the recoil nucleus and the third to the interference term. All of the parameters in the above expression are in the *center of mass* reference frame. The parameter $n_s$ is called the *Sommerfeld parameter* and is given by the expression

$$n_s = \frac{Z^2e^2}{\hbar}\sqrt{\frac{m_{red}}{2E_{lab}}} \quad (17)$$

where $m_{red}$ is the reduced mass of the two nuclides and $E_{lab}$ is the initial beam energy in the lab reference frame.

As evidenced from the expressions (14) and (15), the interference term depends on the spin of the ground state of the colliding nuclei, the initial beam energy, the detection angle and the atomic number (Z) and mass of the nuclei. The type of the spin value (integer or semi-integer number) determines the bosonic or fermionic nature of the nuclei and thus changes the sign of the term, while greater spins lead to a smaller interference contribution. The same is true for the beam energy, as for greater energies the effect of the phenomenon wanes.

Since Mott scattering is a forward scattering process, the detection angle in the c.m. has a range of $0^o < \theta < 180^o$ while in the lab system this range translates to $0^o < \theta < 90^o$. The $0^o$ and $180^o$ degrees are mathematical poles for the expression and so are the $0^o$ and $90^o$ degrees for the Lab system. The scattering is symmetrical around the $90^o$ angle in the c.m. system and around the $45^o$ angle in the lab one. This symmetry in the scattering angle is a result of the reaction kinematics [Canto_14].

It should be noted here that elastic scattering is not the only possible interaction mechanism for two identical colliding nuclei. At low energies, Mott scattering is the main (but not necessarily the only) interaction mechanism, while for energies near or above the Coulomb interaction barrier, nuclear reaction contributions in the differential cross section become important. An indicative interaction barrier for two nuclei with $A_1$, $Z_1$ and $A_2$, $Z_2$ accordingly is given by the expression:

$$U_{Coulomb} = \frac{1.438\, Z_1Z_2}{0.5+1.36\cdot(A_1{}^{1/3}+A_2{}^{1/3})}\ (in\ MeV) \quad (18)$$

where the denominator corresponds to the so-called 'Coulomb radius' and the result is given in the *Center of Mass* reference frame. Other approaches in literature for the interaction barrier include Bass's model, the proximity barrier etc.

## 1.3 Screening Effect

For the theoretical calculations to be able to be compared with experimental results the screening by the electrons shells of both nuclei must be considered. This is achieved via implementing a correction factor, namely the screening factor $f$. The corrected differential cross section for the projectile is given by the expression [Andersen_77]

$$\frac{d\sigma}{d\Omega}_{corrected,projectile} = f_{screening} \frac{d\sigma}{d\Omega}_{projectile} \quad (19)$$

For the determination of the screening factor the Andersen model is adopted which gives the correction for the cross section in the *c.m.* reference frame. According to the model the screening factor is given by the expression [Andersen_77]:

$$f_{Andersen} = \frac{(1+\frac{1}{2}\frac{V_1}{E})^2}{\{1+\frac{V_1}{E}+[\frac{V_1}{2Esin(\frac{\theta}{2})}]^2\}^2} \quad (20)$$

where E and θ are the initial beam energy and the detection angle respectively in the c.m. system. $V_1$ is the increase in the kinetic energy given in keV. This increase is equal to [Andersen_77]:

$$V_1 \text{ (keV)} = 0.04873\ Z_{projectile} Z_{recoil} \sqrt{Z_{projectile}^{2/3} + Z_{recoil}^{2/3}} \quad (21)$$

The corrected differential cross section for the recoil nucleus for detection angle ϕ is calculated via reverse kinematics and is given by the expression [Andersen_77]:

$$\sigma(\varphi_{lab})_{recoil,corrected} = 4 \frac{sin^2(\theta_{lab})\cos(\theta-\theta_{lab})\cos(\varphi_{lab})}{sin^2(\theta)} \sigma(\theta_{lab})_{corrected,scattered} \quad (22)$$

However, in the case of Mott scattering the two nuclei (scattered and recoil) are indistinguishable. Moreover, the parameters that determine the screening factor (velocity, initial energy and detection angle of the nucleus) are the same for both. This allows us to apply the screening factor universally to the Mott differential cross section (including the interference term).

$$\sigma(\theta)_{Mott,corrected} = f(E,\theta)_{Andersen}\, \sigma(\theta)_{Mott} \quad (23)$$

The expression for the screened Mott differential cross section in the lab system is calculated using expression (5). According to it, the cross section in the Lab frame of reference is equal to

$$\sigma(\theta)_{Mott,lab,screened} = \sigma(\theta)_{Mott,cm,screened} \frac{d\Omega_{cm}}{d\Omega_{lab}} \quad (24)$$

It should be noted here that the existing models for the screening effect are all phenomenological in nature. In addition, the accuracy of the Andersen model has certain limitations. The results for small energies (300 keV and lower) and small detection angles (smaller than 20°) should be considered with prudence.

# 2. The Excel Spreadsheet

The main function of the excel spreadsheet is to provide detailed calculations for Mott scattering differential cross sections. In this regard, it allows for the creation of angular or energy distributions of the Mott differential cross section for 314 different isotopes, in both the lab and c.m. reference frames. It also provides comparisons with the corresponding Rutherford values and information about the influence of the screening effect on the calculations. To use the spreadsheet only a few easy steps are required, which are described below.

## 2.1 How to Install

The Excel spreadsheet does not need any installation process once the download is completed. However, for the spreadsheet to be able to function, the user should make sure that in the Excel

- Macros are enabled
- The set decimal separator is the point symbol and not the comma one

The first time the spreadsheet is opened, the user must also enable the function 'Edit content'.

## 2.2 How to Use

The spreadsheet contains 4 different worksheets named Quick Calculation, Angular Distribution, Energy Distribution and Table of Isotopes. The first worksheet, Quick Calculation functions as the point of interaction between the user and the code. In it the user can choose an isotope as incident and target nucleus and specify the characteristics of the distribution. By pressing the buttons "Angular Distribution" or "Energy Distribution" the corresponding distribution appears in the worksheet. It is shown in the *lab system* and it is also presented graphically.

The worksheets Angular Distribution and Energy Distribution show the distribution in both the *lab* and *center of mass* reference frames. Moreover, they offer comparisons with the Rutherford values of the differential cross sections in both systems and the degree of the screening effect for each individual step of the distribution. The above are also presented graphically.

The worksheet Table of Isotopes contains the information about the mass (A), atomic (Z) number, mass and spin of the ground state of the 314 available isotopes (including all the stable and a few radioactive ones). It is possible to expand this list by adding additional isotopes. The functions and contents of each worksheet are presented in detail below.

### *2.2.1 "Quick Calculation" Worksheet*

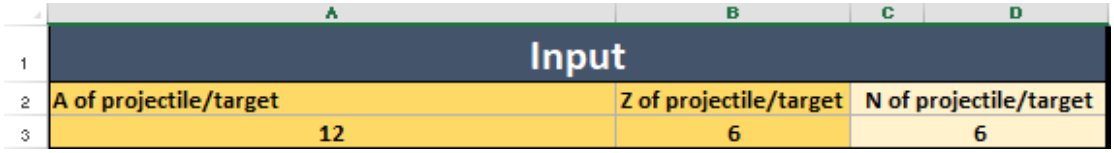
As stated above, this worksheet serves as the point of interaction between the program and the user. To create a distribution the user must follow the following steps:

- Select an isotope to serve as incident and target nucleus
- Select the type of distribution (angular or energy)
- Define the characteristics of the distribution

The cells required for the creation of a distribution are colored bright yellow.

#### *2.2.1.a Selecting an Isotope*

First an isotope needs to be selected to serve both as incident and target nucleus. To select an isotope, simply type the mass number (A) of the isotope in the cell A3 and its atomic number (Z) in cell B3. The program will automatically fill in the number of neutrons of the isotope as well as its mass and ground state spin. For the available isotopes see the worksheet Table of Isotopes. *If the desired isotope is not included in the library a warning will appear informing the user of the fact. The mass and spin of the isotope will be set to zero which will result in false results.* For the addition of isotopes into the library see below.

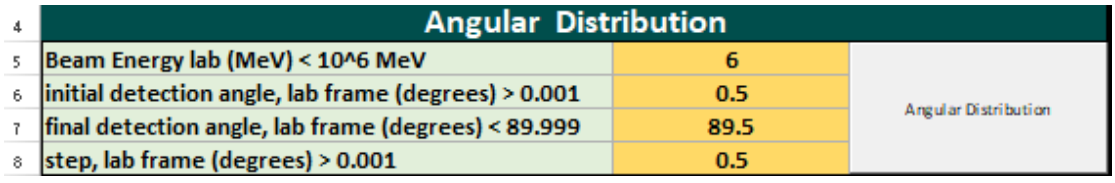


| | A | B | C | D |
|---|---|---|---|---|
| 1 | Input | | | |
| 2 | A of projectile/target | Z of projectile/target | N of projectile/target | |
| 3 | 12 | 6 | 6 | |

**Image 1:** The isotope selection cells in the "Quick Calculation" worksheet. By filling the cells for the mass and atomic number an isotope is selected. If an isotope is not selected then no distribution can be created.

#### *2.2.1.b Selecting and defining a distribution*

After selecting an isotope, the user can specify the characteristics of an angular distribution by filling cells B5 to B8. These characteristics include the beam energy in MeV (cell B5), the initial and final detection angle of the distribution in degrees (cells B6 and B7) and the step between the detection angles (cell B8). Exceeding the suggested limits for these angles (see image 2) will result in *overflow* errors. The limits on the beam energy and the step are based on the limitations of Excel. The limits on the initial and final detection angle originate from the fact that Mott scattering is a forward scattering process where 0 and 90 degrees are mathematical poles. Due to the above, *the program does not allow the user to exceed these limits.*



| | Angular Distribution | | |
|---|---|---|---|
| 5 | Beam Energy lab (MeV) < 10^6 MeV | 6 | Angular Distribution |
| 6 | initial detection angle, lab frame (degrees) > 0.001 | 0.5 | |
| 7 | final detection angle, lab frame (degrees) < 89.999 | 89.5 | |
| 8 | step, lab frame (degrees) > 0.001 | 0.5 | |

**Image 2:** The cells for specifying the characteristics of the angular distribution and their limits for avoiding overflow errors. By pressing the button the distribution is created.

By pressing the button “Angular Distribution” the specified distribution is created, as well as a graphical representation of it in the *lab* reference frame.

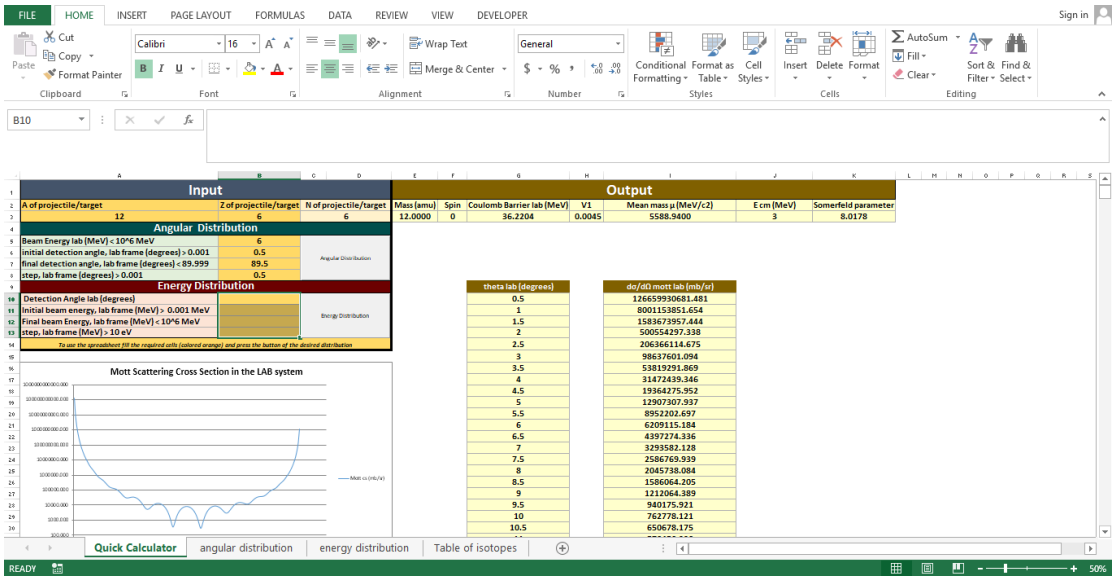



**Image 3:** An image of the worksheet “Quick Calculation”. In the top left corner under the Input label are the cells for the isotope selection and for the characteristics of the angular and energy distributions. By pressing either button, the values of the distribution appear on the worksheet, along with a graph and some additional information.

Along with the distribution some additional information is displayed. More specifically, the mass and spin of the selected isotope, the Coulomb (interaction) barrier of the reaction, the decrease in kinetic energy due to the screening effect ($V_1$), the mean mass of the system, the beam energy in the *c.m.* reference frame and the Sommerfeld parameter.

| Output | | | | | | |
|---|---|---|---|---|---|---|
| Mass (amu) | Spin | Coulomb Barrier lab (MeV) | V1 | Mean mass μ (MeV/c2) | E cm (MeV) | Somerfeld parameter |
| 12.0000 | 0 | 36.2204 | 0.0045 | 5588.9400 | 3 | 8.0178 |

**Image 4:** Additional information shown in the Output panel in the worksheet “Quick Calculator” for an angular distribution.

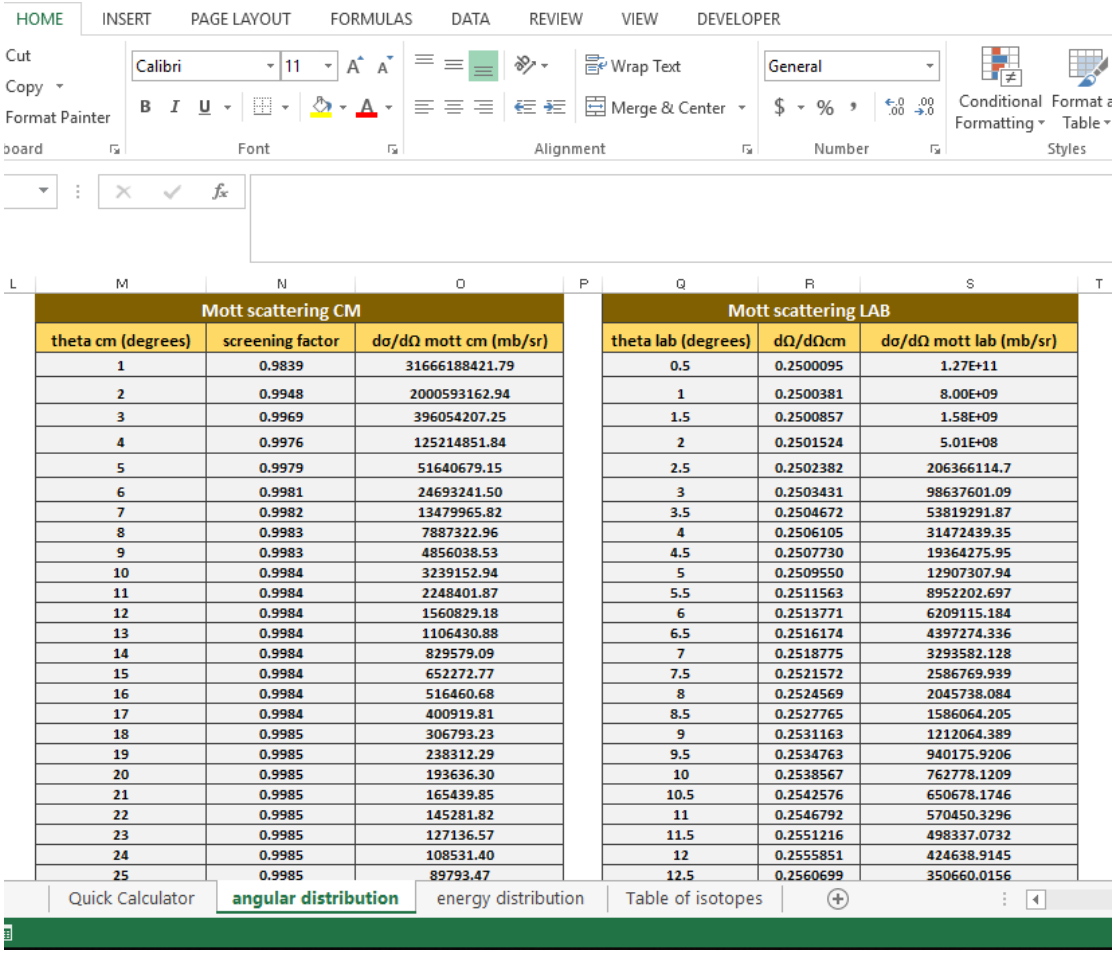
All of the above also apply for the creation of an energy distribution. The user simply fills in the cells B10 to B13 with the characteristics of the distribution and presses the button “Energy Distribution”.

| Energy Distribution | | |
|---|---|---|
| Detection Angle lab (degrees) | 12 | Energy Distribution |
| Initial beam energy, lab frame (MeV) > 0.001 MeV | 1 | |
| Final beam Energy, lab frame (MeV) < 10^6 MeV | 10 | |
| step, lab frame (MeV) > 10 eV | 0.1 | |
| *To use the spreadsheet fill the required cells (colored orange) and press the button of the desired distribution* | | |

**Image 5:** The cells for specifying the characteristics of the energy distribution and their limits for avoiding overflow errors. By pressing the button the distribution is created.

*2.2.2 "Angular Distribution" and "Energy Distribution" Worksheets*

The worksheets "Angular Distribution" and "Energy Distribution" hold additional information for the corresponding distribution. There, the cross section values for Mott scattering in both the *lab and c.m.* reference frames are stored. Moreover, the influence of the screening effect (called screening factor) and the value $d\Omega/d\Omega_{cm}$, which is used to change the value of the cross section from the *c.m.* reference frame to the *lab one*, can be found there.

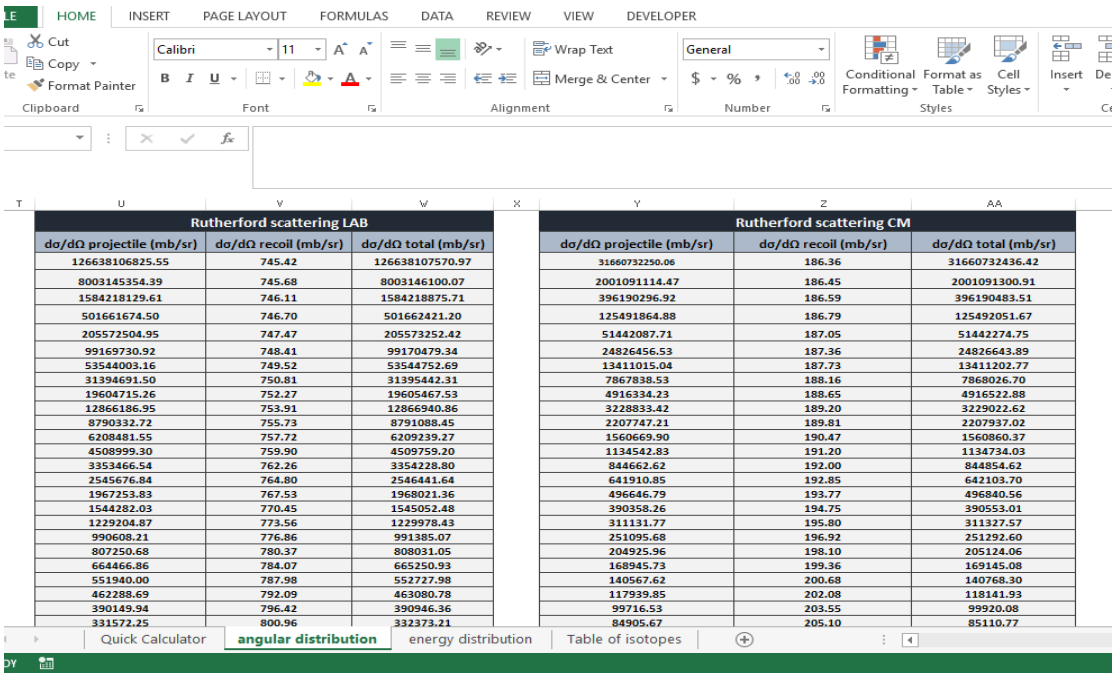


| Mott scattering CM | | |
|---|---|---|
| theta cm (degrees) | screening factor | dσ/dΩ mott cm (mb/sr) |
| 1 | 0.9839 | 31666188421.79 |
| 2 | 0.9948 | 2000593162.94 |
| 3 | 0.9969 | 396054207.25 |
| 4 | 0.9976 | 125214851.84 |
| 5 | 0.9979 | 51640679.15 |
| 6 | 0.9981 | 24693241.50 |
| 7 | 0.9982 | 13479965.82 |
| 8 | 0.9983 | 7887322.96 |
| 9 | 0.9983 | 4856038.53 |
| 10 | 0.9984 | 3239152.94 |
| 11 | 0.9984 | 2248401.87 |
| 12 | 0.9984 | 1560829.18 |
| 13 | 0.9984 | 1106430.88 |
| 14 | 0.9984 | 829579.09 |
| 15 | 0.9984 | 652272.77 |
| 16 | 0.9984 | 516460.68 |
| 17 | 0.9984 | 400919.81 |
| 18 | 0.9985 | 306793.23 |
| 19 | 0.9985 | 238312.29 |
| 20 | 0.9985 | 193636.30 |
| 21 | 0.9985 | 165439.85 |
| 22 | 0.9985 | 145281.82 |
| 23 | 0.9985 | 127136.57 |
| 24 | 0.9985 | 108531.40 |
| 25 | 0.9985 | 89793.47 |

| Mott scattering LAB | | |
|---|---|---|
| theta lab (degrees) | dΩ/dΩcm | dσ/dΩ mott lab (mb/sr) |
| 0.5 | 0.2500095 | 1.27E+11 |
| 1 | 0.2500381 | 8.00E+09 |
| 1.5 | 0.2500857 | 1.58E+09 |
| 2 | 0.2501524 | 5.01E+08 |
| 2.5 | 0.2502382 | 206366114.7 |
| 3 | 0.2503431 | 98637601.09 |
| 3.5 | 0.2504672 | 53819291.87 |
| 4 | 0.2506105 | 31472439.35 |
| 4.5 | 0.2507730 | 19364275.95 |
| 5 | 0.2509550 | 12907307.94 |
| 5.5 | 0.2511563 | 8952202.697 |
| 6 | 0.2513771 | 6209115.184 |
| 6.5 | 0.2516174 | 4397274.336 |
| 7 | 0.2518775 | 3293582.128 |
| 7.5 | 0.2521572 | 2586769.939 |
| 8 | 0.2524569 | 2045738.084 |
| 8.5 | 0.2527765 | 1586064.205 |
| 9 | 0.2531163 | 1212064.389 |
| 9.5 | 0.2534763 | 940175.9206 |
| 10 | 0.2538567 | 762778.1209 |
| 10.5 | 0.2542576 | 650678.1746 |
| 11 | 0.2546792 | 570450.3296 |
| 11.5 | 0.2551216 | 498337.0732 |
| 12 | 0.2555851 | 424638.9145 |
| 12.5 | 0.2560699 | 350660.0156 |

**Image 6:** The columns for the Mott scattering cross sections in the worksheet "Angular Distribution", in the lab and c.m. reference frames. The value $d\Omega/d\Omega_{cm}$ changes for each different angle of detection but the Sommerfeld parameter remains constant, since it depends on the beam energy.

Additionally, the corresponding Rutherford scattering differential cross section values are available in both systems. The values for these cross sections correspond to the same angles or energies as the Mott values.



| Rutherford scattering LAB | | |
|---|---|---|
| dσ/dΩ projectile (mb/sr) | dσ/dΩ recoil (mb/sr) | dσ/dΩ total (mb/sr) |
| 126638106825.55 | 745.42 | 126638107570.97 |
| 8003145354.39 | 745.68 | 8003146100.07 |
| 1584218129.61 | 746.11 | 1584218875.71 |
| 501661674.50 | 746.70 | 501662421.20 |
| 205572504.95 | 747.47 | 205573252.42 |
| 99169730.92 | 748.41 | 99170479.34 |
| 53544003.16 | 749.52 | 53544752.69 |
| 31394691.50 | 750.81 | 31395442.31 |
| 19604715.26 | 752.27 | 19605467.53 |
| 12866186.95 | 753.91 | 12866940.86 |
| 8790332.72 | 755.73 | 8791088.45 |
| 6208481.55 | 757.72 | 6209239.27 |
| 4508999.30 | 759.90 | 4509759.20 |
| 3353466.54 | 762.26 | 3354228.80 |
| 2545676.84 | 764.80 | 2546441.64 |
| 1967253.83 | 767.53 | 1968021.36 |
| 1544282.03 | 770.45 | 1545052.48 |
| 1229204.87 | 773.56 | 1229978.43 |
| 990608.21 | 776.86 | 991385.07 |
| 807250.68 | 780.37 | 808031.05 |
| 664466.86 | 784.07 | 665250.93 |
| 551940.00 | 787.98 | 552727.98 |
| 462288.69 | 792.09 | 463080.78 |
| 390149.94 | 796.42 | 390946.36 |
| 331572.25 | 800.96 | 332373.21 |

| Rutherford scattering CM | | |
|---|---|---|
| dσ/dΩ projectile (mb/sr) | dσ/dΩ recoil (mb/sr) | dσ/dΩ total (mb/sr) |
| 31660732250.06 | 186.36 | 31660732436.42 |
| 2001091114.47 | 186.45 | 2001091300.91 |
| 396190296.92 | 186.59 | 396190483.51 |
| 125491864.88 | 186.79 | 125492051.67 |
| 51442087.71 | 187.05 | 51442274.75 |
| 24826456.53 | 187.36 | 24826643.89 |
| 13411015.04 | 187.73 | 13411202.77 |
| 7867838.53 | 188.16 | 7868026.70 |
| 4916334.23 | 188.65 | 4916522.88 |
| 3228833.42 | 189.20 | 3229022.62 |
| 2207747.21 | 189.81 | 2207937.02 |
| 1560669.90 | 190.47 | 1560860.37 |
| 1134542.83 | 191.20 | 1134734.03 |
| 844662.62 | 192.00 | 844854.62 |
| 641910.85 | 192.85 | 642103.70 |
| 496646.79 | 193.77 | 496840.56 |
| 390358.26 | 194.75 | 390553.01 |
| 311131.77 | 195.80 | 311327.57 |
| 251095.68 | 196.92 | 251292.60 |
| 204925.96 | 198.10 | 205124.06 |
| 168945.73 | 199.36 | 169145.08 |
| 140567.62 | 200.68 | 140768.30 |
| 117939.85 | 202.08 | 118141.93 |
| 99716.53 | 203.55 | 99920.08 |
| 84905.67 | 205.10 | 85110.77 |

Quick Calculator | angular distribution | energy distribution | Table of isotopes

**Image 7:** The columns for the Rutherford scattering differential cross sections in the worksheet "Angular Distribution", in the lab and c.m. reference frames. The total differential cross section is the sum of the projectile and recoil cross sections, excluding any interference term.

Visual comparison between Mott and Rutherford differential cross section values is also available. By pressing the button "Graphs" two graphs are created, comparing Mott and Rutherford cross sections in both systems.

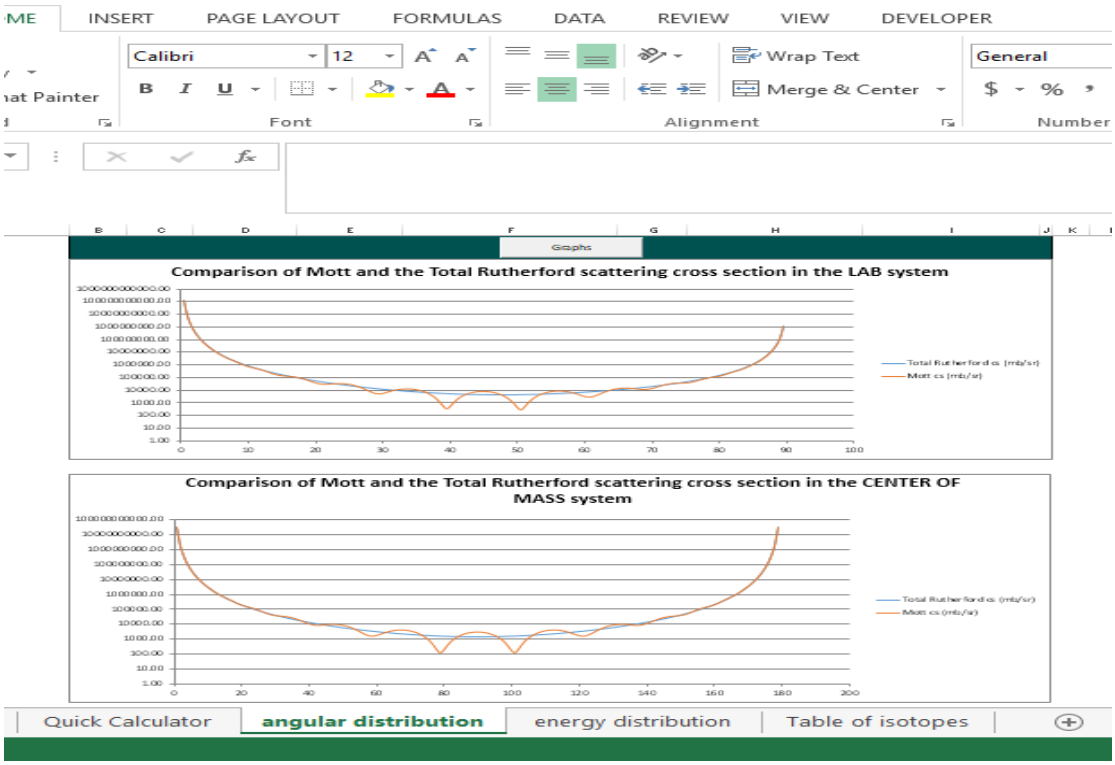



**Image 8:** The graphs comparing the cross section values for Mott (blue) and Rutherford (orange) scattering in the "Angular Distribution" worksheet. The graphs are created only when the button "Graphs" is pressed.

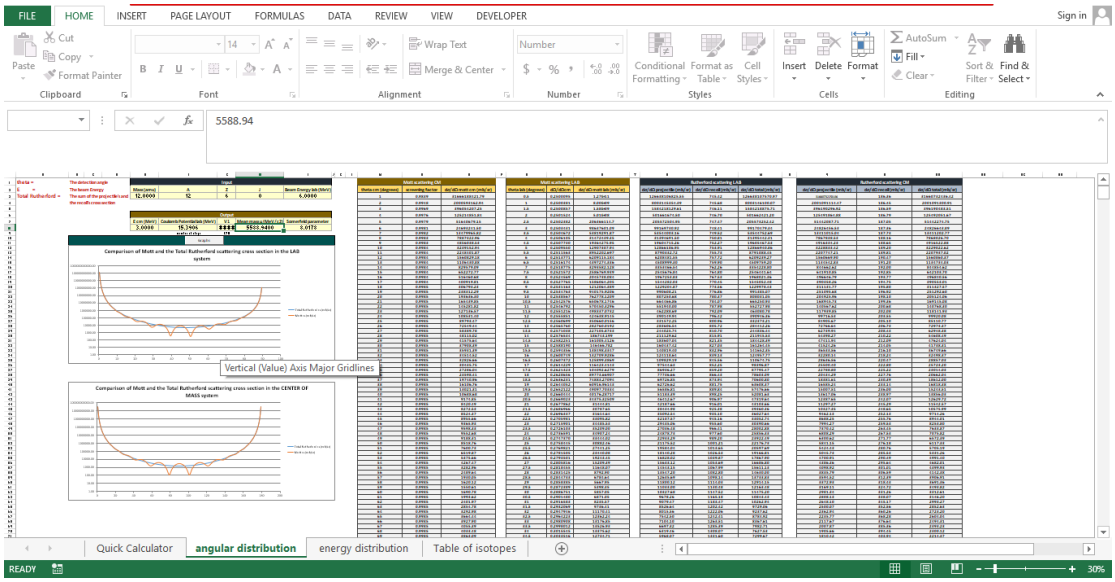



**Image 9:** The full worksheet "Angular Distribution" with the Mott and Rutherford cross section values in both lab and c.m. systems along with the accompanying graphs.

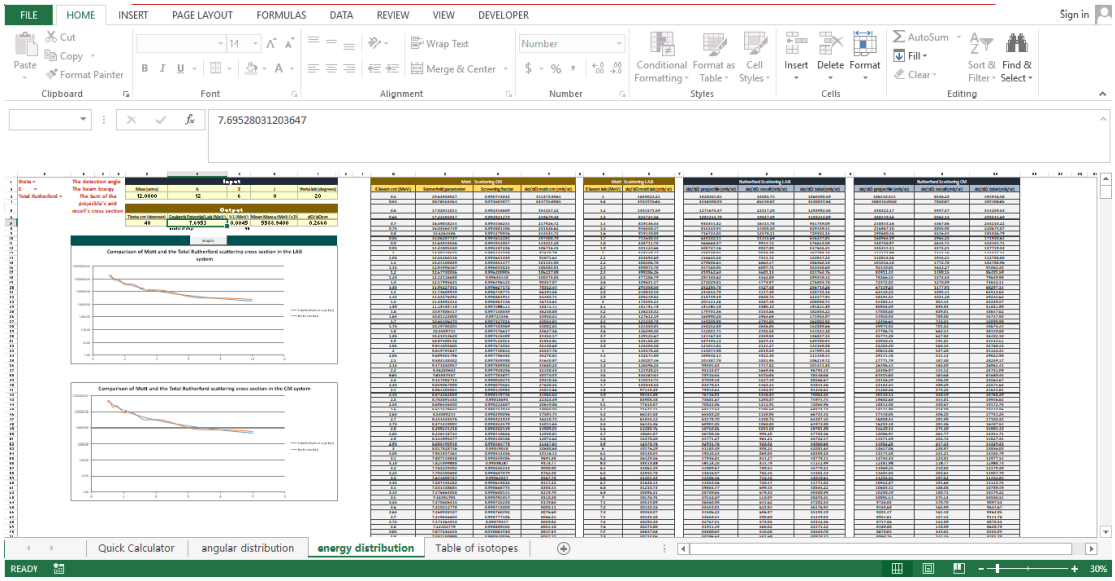
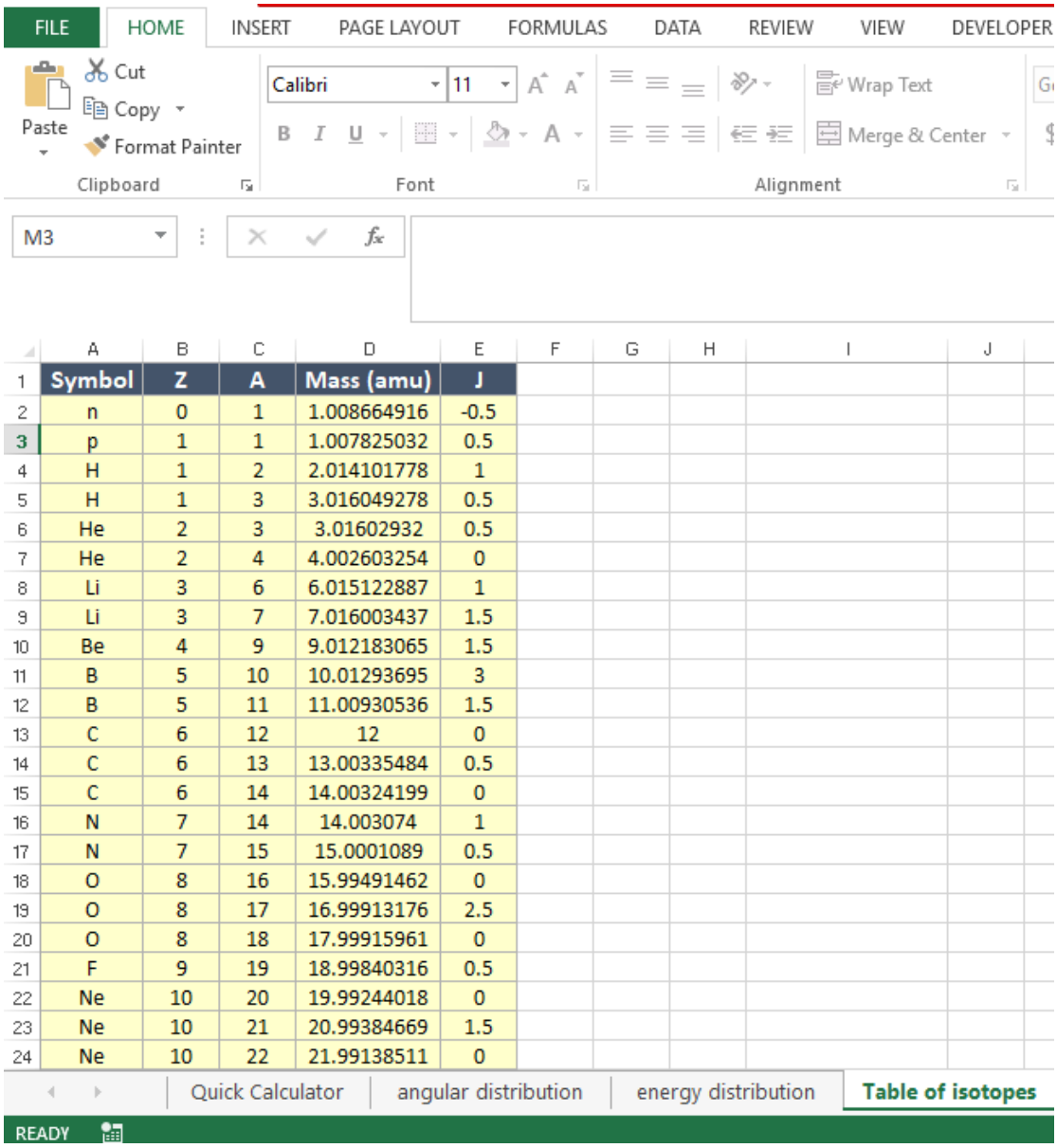



**Image 10:** The full worksheet "Energy Distribution" with the Mott and Rutherford cross section values in both lab and c.m. systems along with the accompanying graphs. In an energy distribution, the value $d\Omega/d\Omega_{cm}$ remains constant, since there is only one detection angle, however the Sommerfeld parameter changes according to the beam energy.

*2.2.3 "Table of Isotopes" Worksheet – Adding an isotope*

The worksheet "Table of Isotopes" contains the 314 available stable (and a few key radioactive) isotopes that the user can choose as projectile and target nuclei. It is made up of 5 columns where the symbol, atomic number (Z), mass number (A), mass and spin of each isotope is stored. The worksheet functions as a library from which the program takes the necessary information for every isotope. This is the reason why this worksheet is locked, to prevent any accidental changes in the isotope database.




| | A | B | C | D | E | F | G | H | I | J |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Symbol | Z | A | Mass (amu) | J | | | | | |
| 2 | n | 0 | 1 | 1.008664916 | -0.5 | | | | | |
| 3 | p | 1 | 1 | 1.007825032 | 0.5 | | | | | |
| 4 | H | 1 | 2 | 2.014101778 | 1 | | | | | |
| 5 | H | 1 | 3 | 3.016049278 | 0.5 | | | | | |
| 6 | He | 2 | 3 | 3.01602932 | 0.5 | | | | | |
| 7 | He | 2 | 4 | 4.002603254 | 0 | | | | | |
| 8 | Li | 3 | 6 | 6.015122887 | 1 | | | | | |
| 9 | Li | 3 | 7 | 7.016003437 | 1.5 | | | | | |
| 10 | Be | 4 | 9 | 9.012183065 | 1.5 | | | | | |
| 11 | B | 5 | 10 | 10.01293695 | 3 | | | | | |
| 12 | B | 5 | 11 | 11.00930536 | 1.5 | | | | | |
| 13 | C | 6 | 12 | 12 | 0 | | | | | |
| 14 | C | 6 | 13 | 13.00335484 | 0.5 | | | | | |
| 15 | C | 6 | 14 | 14.00324199 | 0 | | | | | |
| 16 | N | 7 | 14 | 14.003074 | 1 | | | | | |
| 17 | N | 7 | 15 | 15.0001089 | 0.5 | | | | | |
| 18 | O | 8 | 16 | 15.99491462 | 0 | | | | | |
| 19 | O | 8 | 17 | 16.99913176 | 2.5 | | | | | |
| 20 | O | 8 | 18 | 17.99915961 | 0 | | | | | |
| 21 | F | 9 | 19 | 18.99840316 | 0.5 | | | | | |
| 22 | Ne | 10 | 20 | 19.99244018 | 0 | | | | | |
| 23 | Ne | 10 | 21 | 20.99384669 | 1.5 | | | | | |
| 24 | Ne | 10 | 22 | 21.99138511 | 0 | | | | | |

**Image 11:** The Table of Isotopes worksheet where the information for each available isotope is stored.

It is possible to expand the list of isotopes with additional unstable (RIB) isotopes as the state of the nucleus does not affect the theoretical calculations. First, the user must use the password ***MottCalc*** to unlock the worksheet. Then the five columns must be filled with the characteristics of the new isotope. It can be placed anywhere in the list. Once the isotope has been added to the list, some changes must be made to the code of the spreadsheet.

By clicking on the 'developer' tab, then on 'design mode' and finally double clicking the button "Angular distribution" or "Energy distribution", in the "Quick Calculator" worksheet, access to the code is permitted.

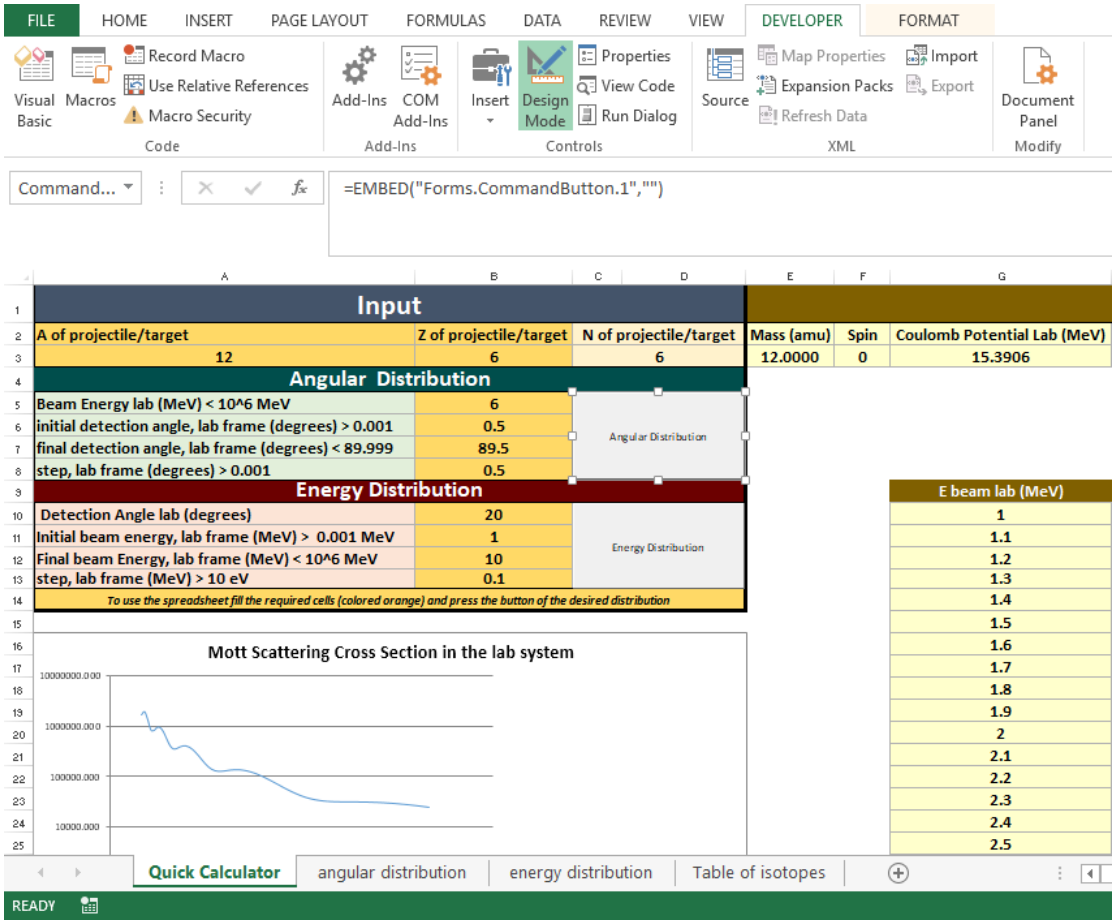



**Image 12:** When 'design mode' is enabled (by clicking on the icon in the developer tab) all the buttons are disabled. By double clicking on them a new window pops up with the code that controls the actions of the button.

A new window will appear with the code behind the spreadsheet. There, in two of the loops labeled as *"change here for addition of isotope"* the user must change the "for" loop from

*For i = 2 To 315*

*to*

*For i = 2 To 316*

And then press the save icon for the changes to be applied.

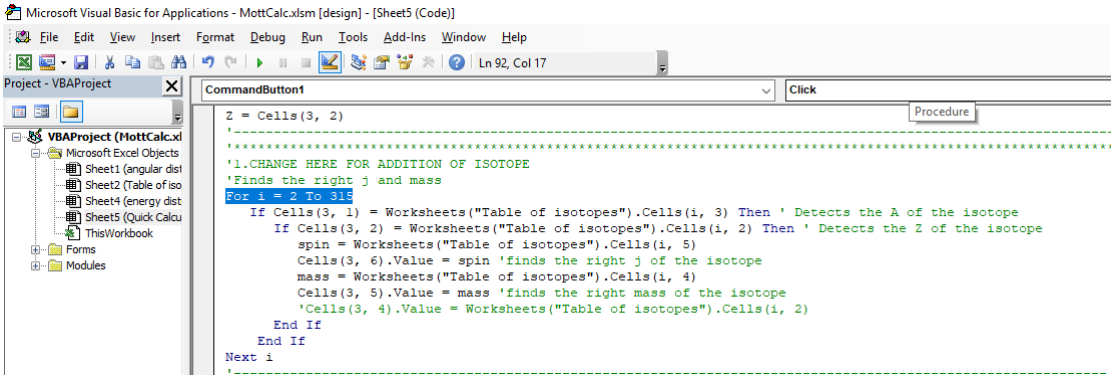



**Image 13:** The new window with the code of the Excel spreadsheet that appears after clicking on any of the buttons in the ”Quick Calculator” worksheet after ‘design mode’ has been enabled.

It is paramount to apply the change to both “for” loops. If not, it is possible that the buttons “Angular Distribution” or “Energy Distribution” will not be able to use the added isotope. To return to normal functionality, the ‘design mode’ must be unclicked.

# 3. The MottCalc Application

MottCalc is also available as a stand-alone application which produces ASCII R33 files with the specified distributions. These files are compatible with all the widely used analytical codes (e.g. SIMNRA, DF etc.). The same methodology for the theoretical calculations as in the Excel spreadsheet is used in the application, however, the software provides only the specified distribution (angular or energy) in the lab reference frame. The same 314 isotopes are available as projectile and target nuclei with the additional ability for the user to create custom isotopes. Instructions on how to install and use the application follow below.

## 3.1 How to Install

When the download is completed please open the Mottcalc-Release.rar file. Extract the file named MottCalc-Release in your hard drive (C:\) or any directory within. The file MottCalc-Release contains essential .dll files without which the program is unable to run. Also, there is a text file included, named TableOfIsotopes.txt, which contains the information concerning the 314 isotopes available as projectile and target nuclei. Last but not least, the executable file is named MottCalc.exe. To run the program just doubleclick the MottCalc.exe file. To ensure the correct operation of the program the following must be true:

- The files MottCalc.exe and TableOfIsotopes.txt are located in the MottCalc-Release file along with all the .dll files.
- The filepath to the directory of the MottCalc-Release file does not contain any special characters (for example characters from non-Latin alphabets).

If any of the above is not true then the executable will not be able to locate the TableOfIsotopes.txt file. In other words, the program will not have access to its isotope library.

## 3.2 How to Use

Once the program window appears, to create a distribution the user must

- select an isotope to act as projectile and target nucleus
- select a mode defining the distribution type (angular or energy)
- define the characteristics of the distribution

When the above steps are completed, a graph of the distribution is generated and the values of the distribution are stored in the computer memory. At this point the user has the option to save the generated distribution in an ASCII R33 format file.

### *3.2.1 Selecting an Isotope*

There are two choices for setting an isotope as projectile and target nucleus. Firstly, there exist the 314 available isotopes in the program library. To choose one of them, the boxes A and Z must be filled in the tab "Select Isotope from the Library" and then the button "Set Isotope" must be pressed. When the button is pressed the grey boxes labeled "mass" and "spin" will show the correct mass and spin of the selected isotope and the isotope information is stored in the computer memory. To change the selected isotope, the same methodology must be followed. It is paramount to note that the new isotope will not be selected by just changing the values of the "A" and "Z" boxes. The button "Set Isotope" must be pressed every time for the change to take effect, else the new isotope will not replace the old one in the memory.

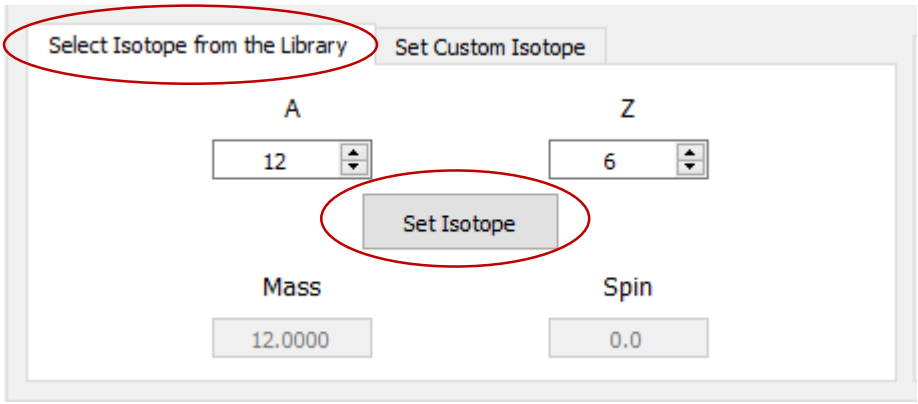



**Image 14:** The "Select Isotope from the Library" tab. To select an isotope, the A and Z labeled boxes must be filled and the "Set Isotope" button pressed. In the present example the selected isotope is the stable nucleus $^{12}C$.

If the specified isotope is not included in the library a warning will appear and the mass of the nucleus will be set to 0.0100 and its spin to 0. If an isotope is not selected, the user cannot create a distribution. The available isotopes are stored in the TableOfIsotopes.txt file.

To use an isotope not included in the library, the "Set Custom Isotope" tab must be used. To create a custom isotope, in addition to its mass (A) and atomic (Z) numbers its precise mass and spin must also be specified. Again, if the button "Set Isotope" is not pressed, the custom isotope will not be selected. The program cannot determine the validity (nor even the actual existence) of the custom isotopes.

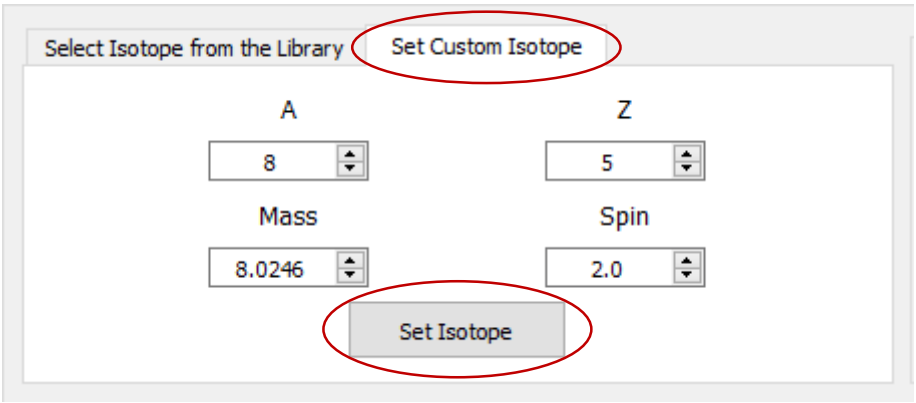



**Image 15:** The "Set Custom Isotope" tab. To select an isotope the A, Z, mass and spin labeled boxes must be filled and the "Set Isotope" button pressed. In the present example the custom isotope is the unstable nucleus $^{8}B$.

### *3.2.2 Selecting a Mode*

Once an isotope has been selected, the type of the distribution must be selected as well from the "Mode Selection" box. Selecting "Angular Distribution" or "Energy Distribution" allows the user to specify the characteristics of each distribution. For an angular distribution these are the beam energy, its initial and final detection angles and the angular step. For an energy distribution the characteristics are the detection angle, the initial and final beam energies and the energy step.

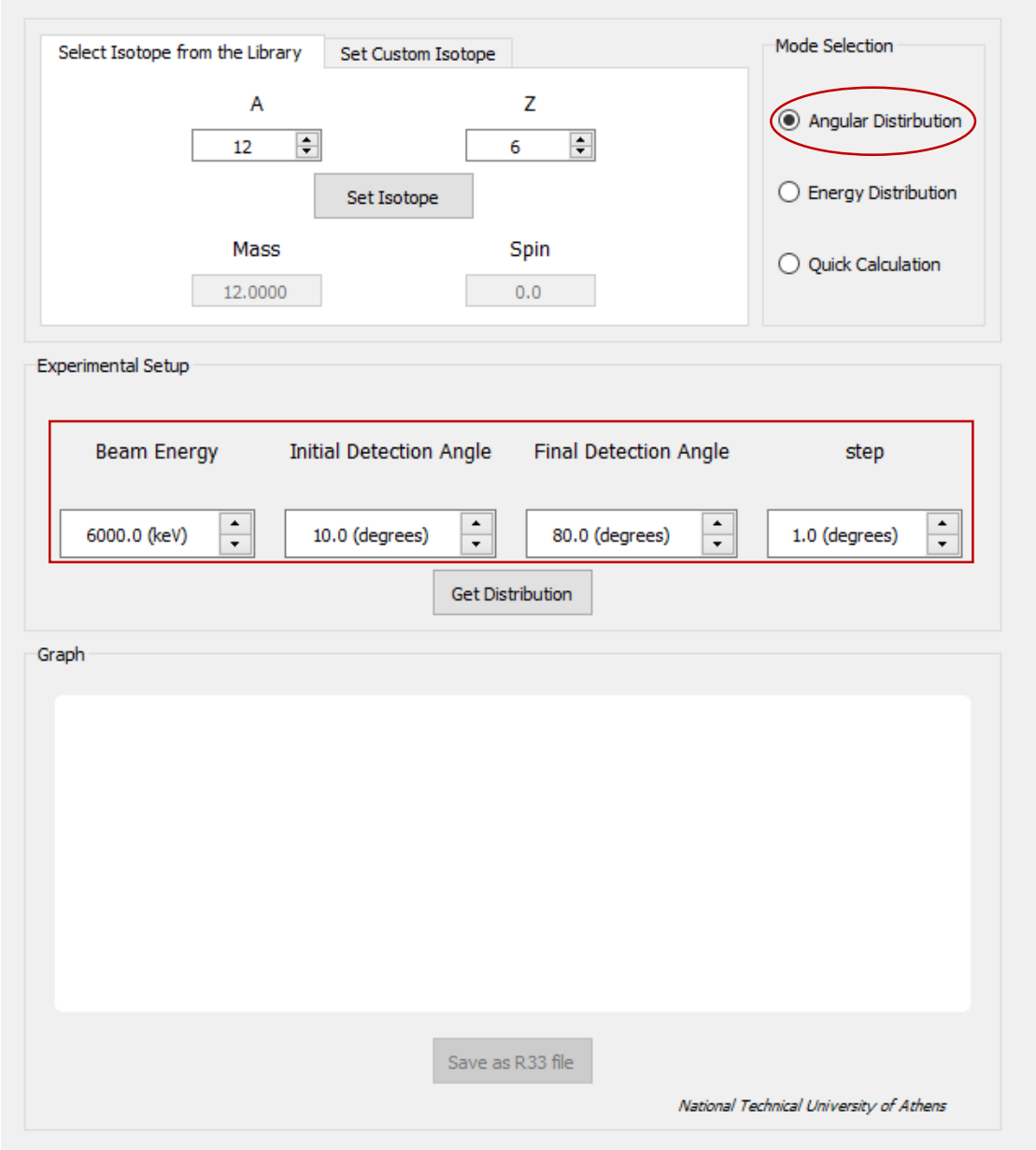



**Image 16:** Once a Mode has been selected (red circle) the user is able to specify the characteristics of a distribution. For an angular distribution these are the beam energy, the initial and final detection angle and the angular step (red rectangle).

By pressing the "Get Distribution" button the distribution is created along with a graph, and stored in the program memory. To create a new distribution, along with the changes in its characteristics, the "Get Distribution" button must be pressed again. If the button is not pressed, the new distribution will not replace the old one in the memory and in the graph.

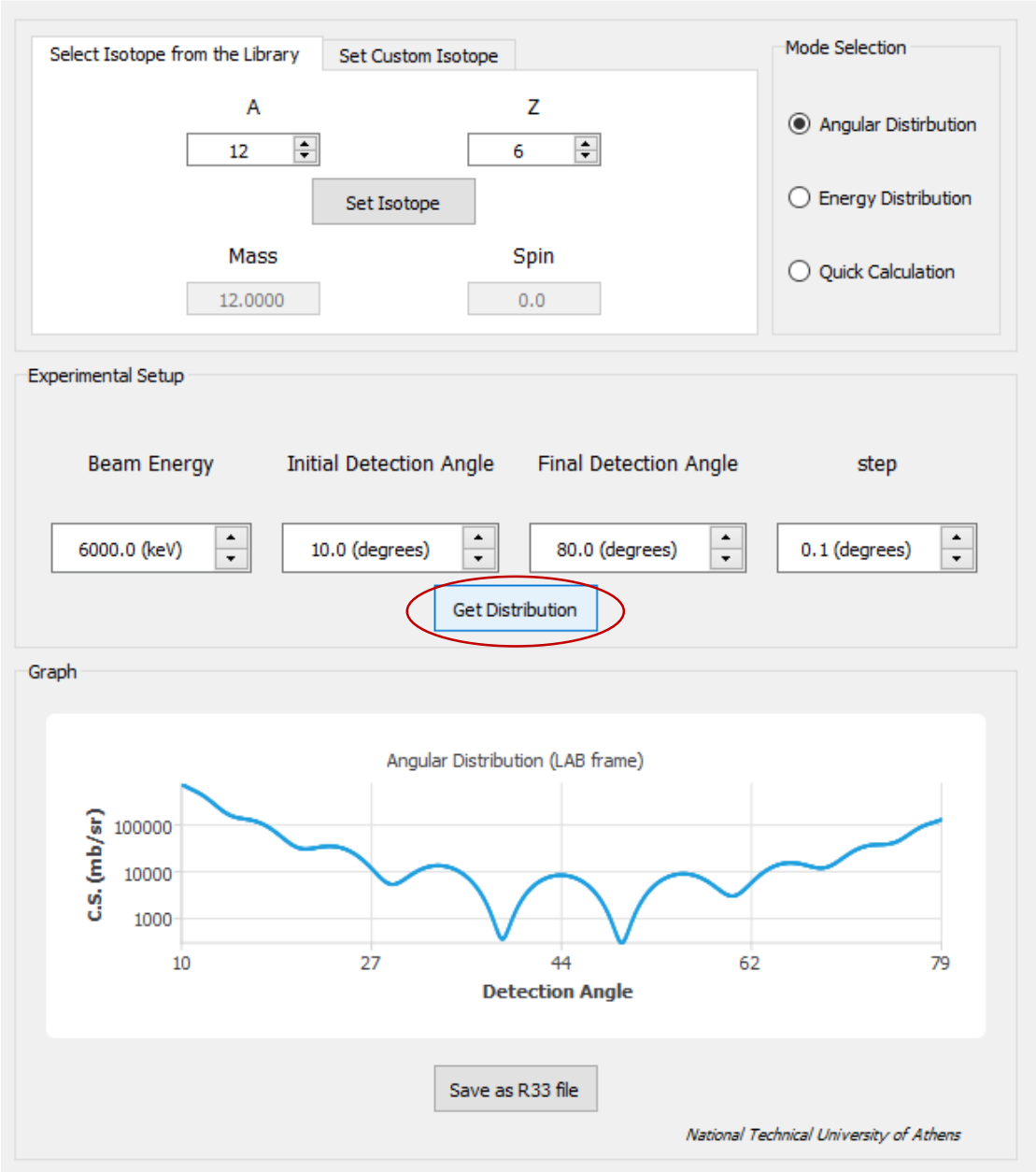



**Image 17:** By pressing the "Get Distribution" button (red circle) the specified distribution is created and stored in the memory. A graph of the distribution is also generated.

The “Quick Calculation” mode is different from the other two, since it does not generate a distribution. This mode allows for the calculation of the differential cross section of Mott scattering for a specific detection angle and beam energy combination.

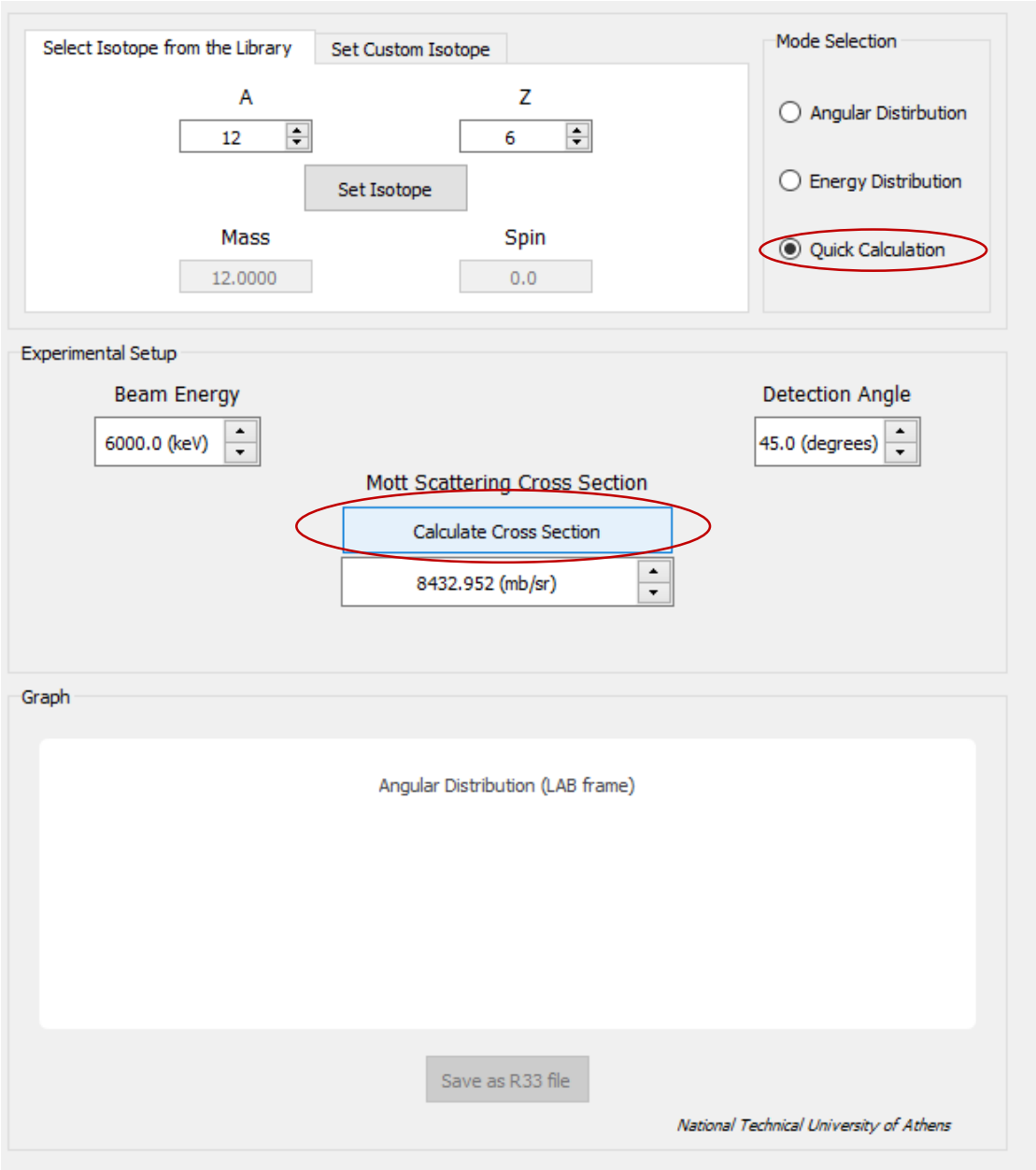



**Image 18:** The mode “Quick Calculation” allows for the calculation of Mott scattering differential cross section for a specific detection angle and beam energy combination.

### *3.2.3 Creating an R33 file*

Once the distribution is created, the user can save it in an ASCII R33 file format by pressing the “Save as R33 File” button. By pressing the button the user can choose where the R33 file will be stored and under which name.

# 4. References


| | |
|---|---|
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