NORTHERN ILLINOIS UNIVERSITY

PHYSICS DEPARTMENT

Physics 580 – Solid State Physics Fall 2022

Problem Set #4

Bring laptop with Python installed on Tues (see Problem #6)
Problem Set Due: Thurs, Sept. 29, 2022 (have Problem #1 and Python done by Tues)
Read Kittel: Chapter 2, powerpoint: *X-ray Diffraction*

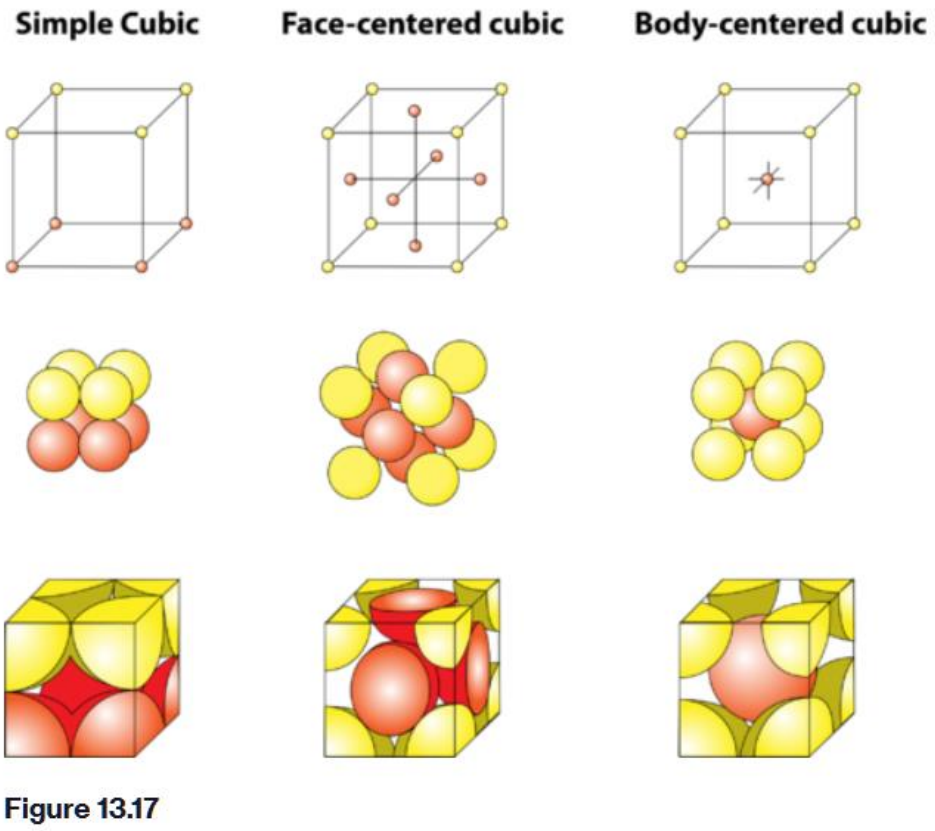
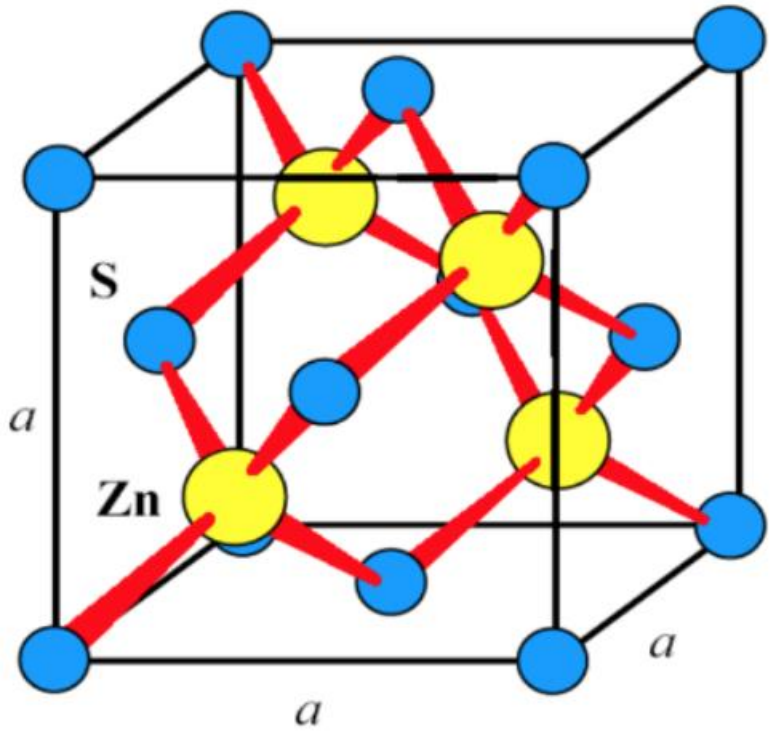


Figure 13.17

from webpage: https://www.coursehero.com/study-guides/cheminter/unit-cells/

1. Gold crystallizes in a cubic close-packed structure (face-centered cubic unit cell) and has a density of 19.3 g/cm^3. Calculate the atomic radius of an Au atom in angstroms (Å). Use only these values, Avogadro's number, and the molecular weight (or molar mass) of Au from the periodic table of the elements. Assume the atoms pack the unit cell as shown the two lower rows in the figure above (the atoms are modeled as spheres in contact with each other). How does your value compare with the actual atomic radius of gold in an fcc structure? (Google this value, and answer in % larger or smaller).



2. ZnS crystallizes into what is referred to as a zincblende structure. The zincblende structure is an fcc lattice with a diatomic base with one atom at (0, 0, 0) and the other atom at (¼, ¼, ¼). The atoms are tetrahedrally coordinated, each atom having four neighboring atoms.

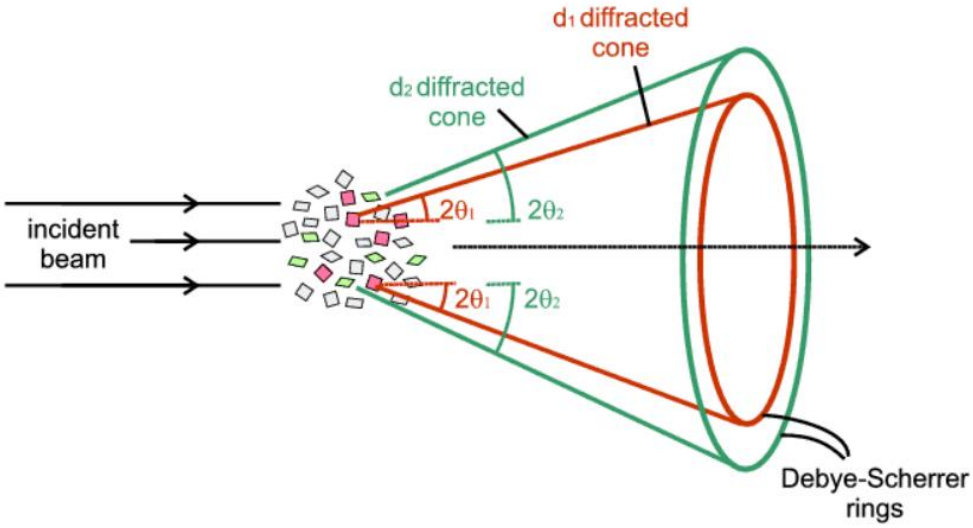
   (a) How many of each atom are contained within a unit cell of ZnS?

   (b) Many types of compounds crystallizes into the zincblende structure: BP (boron phosphide), ZnTe (zinc telluride), GaAs (gallium arsenide), MgSe (mercury selenide), to name a few. What is the difference between the diamond structure and the zincblende structure? (that is, why is the diamond crystal structure not called the zincblende structure?)

3. The edge length of the NaCl unit cell is 5.64 Å. Determine the density of NaCl in g/cm^3 using the molecular weight of Na and Cl from the periodic table of the elements and Avogadro's number. Make certain it agrees with the value given in Wikipedia (what is this value, and does your answer agree with it?).

4. Read through the powerpoint *X-ray Diffraction* located on Blackboard (in the "Content" section).

   (a) Write down Bragg's law with the Miller indices in mind as is done in the *X-ray Diffraction* powerpoint.



   from webpage: http://pd.chem.ucl.ac.uk/pdnn/diff2/kinemat2.htm

   (b) Why does a polycrystalline material (see figure above) give rise to Debye-Scherrer rings for diffracted x-ray beams.

5. Kittel: **Problem 5** (see below)

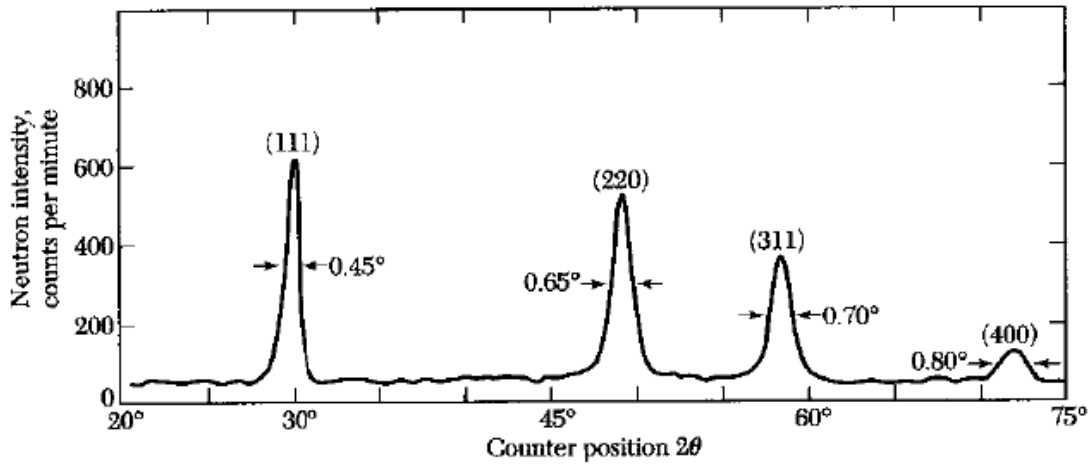


Figure 18 Neutron diffraction pattern for powdered diamond. (After C. Bacon.)

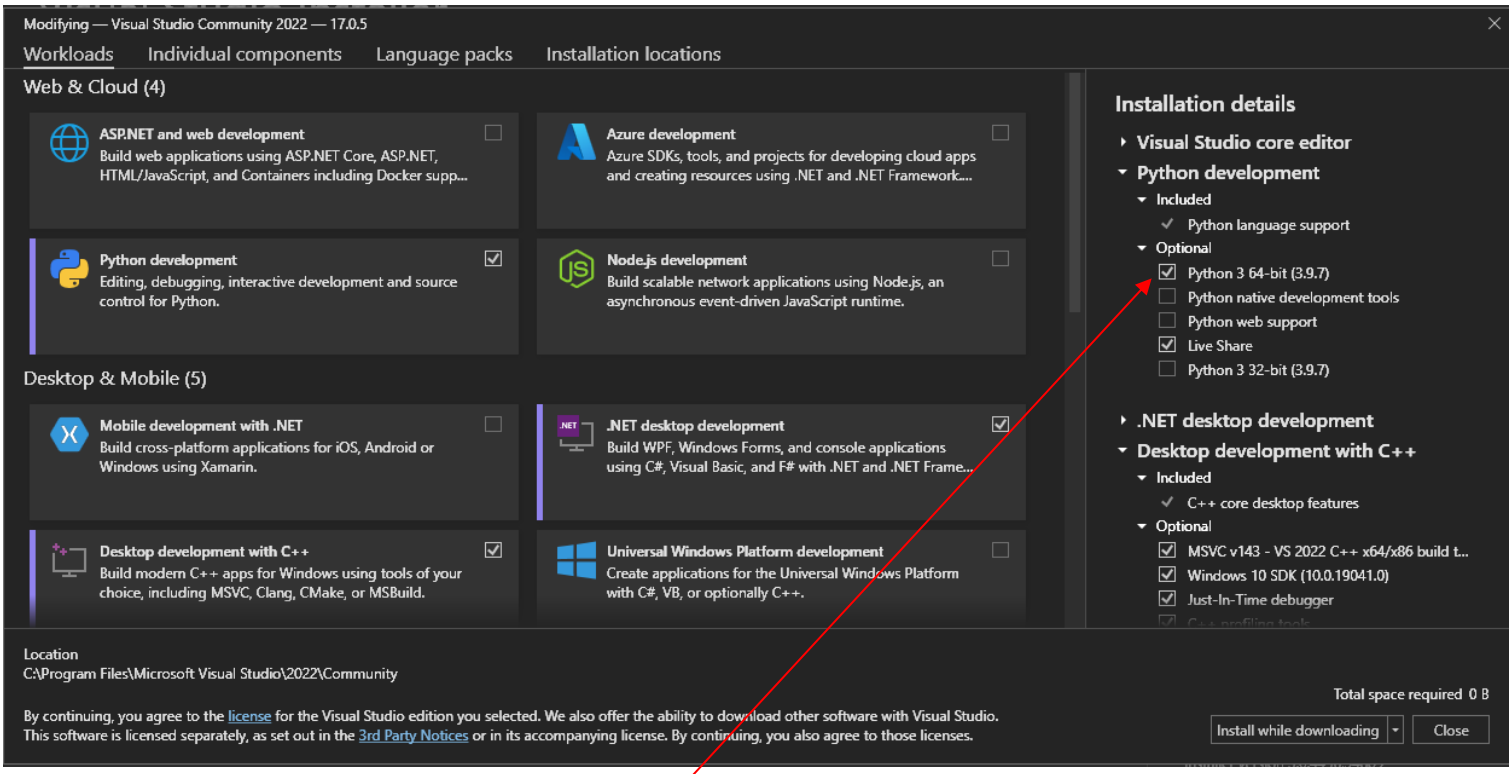
5. ***Structure factor of diamond.*** The crystal structure of diamond is described in Chapter 1. The basis consists of eight atoms if the cell is taken as the conventional cube. (a) Find the structure factor S of this basis. (b) Find the zeros of S and show that the allowed reflections of the diamond structure satisfy $v_1 + v_2 + v_3 = 4n$, where all indices are even and n is any integer, or else all indices are odd (Fig. 18). (Notice that h, k, l may be written for v_1, v_2, v_3 and this is often done.)

6. Install Python and Microsoft Visual Studio Community on your laptop (if you do not have these already). You can follow the instructions in the tutorial below. At the end, you will write a simple Python program: "hello world".

Installation of Python

The version of Python used in this Tutorial is Python 3.7. The integrated development environment (IDE) that is used is Microsoft Visual Community 2022 (available for both the PC and the MAC). Installing Microsoft Visual Community is free will also install Python if you do not have a version installed.

Do a Google search for Microsoft Visual Community and install it by selecting the following additional features (they are not installed by default): (1) Python development and (2) Desktop development with C++. If desired, you can install other packages (like the Visual Basic package selected below).



Make certain to select "*Python 3 64-bit*" (it is not selected by default) if you do not have Python already installed on your system.

Python is a dynamic language (executed by an interpreter) that cannot be compiled into machine code statically (like C++ and Fortran). It is an interpreter programming language that is needed to execute Python commands.

Fortunately, *pip* is installed automatically when Python is installed. If pip is not installed, go to: https://pip.pypa.io/en/stable/installation/. If you get a warning that a newer version of pip is available then you should upgrade. To do this, (*for a PC*) click on the Start button and type "powershell" and select the Windows PowerShell application. In PowerShell type:

```
py -m pip install --upgrade pip
```

If you get a warning that a Python Scripts directory are not on PATH, add the directory to PATH by editing the system environment variables. Documentation can be found at:

https://www.architectryan.com/2018/03/17/add-to-the-path-on-windows-10/

To add the Scripts directory to PATH: (1) click on the Start button and type "env", then select "Edit the system environment variables", (2) select the "Advanced" tab, (3) click the "Environment Variables…" button, (4) Under the "System Variables" section (the

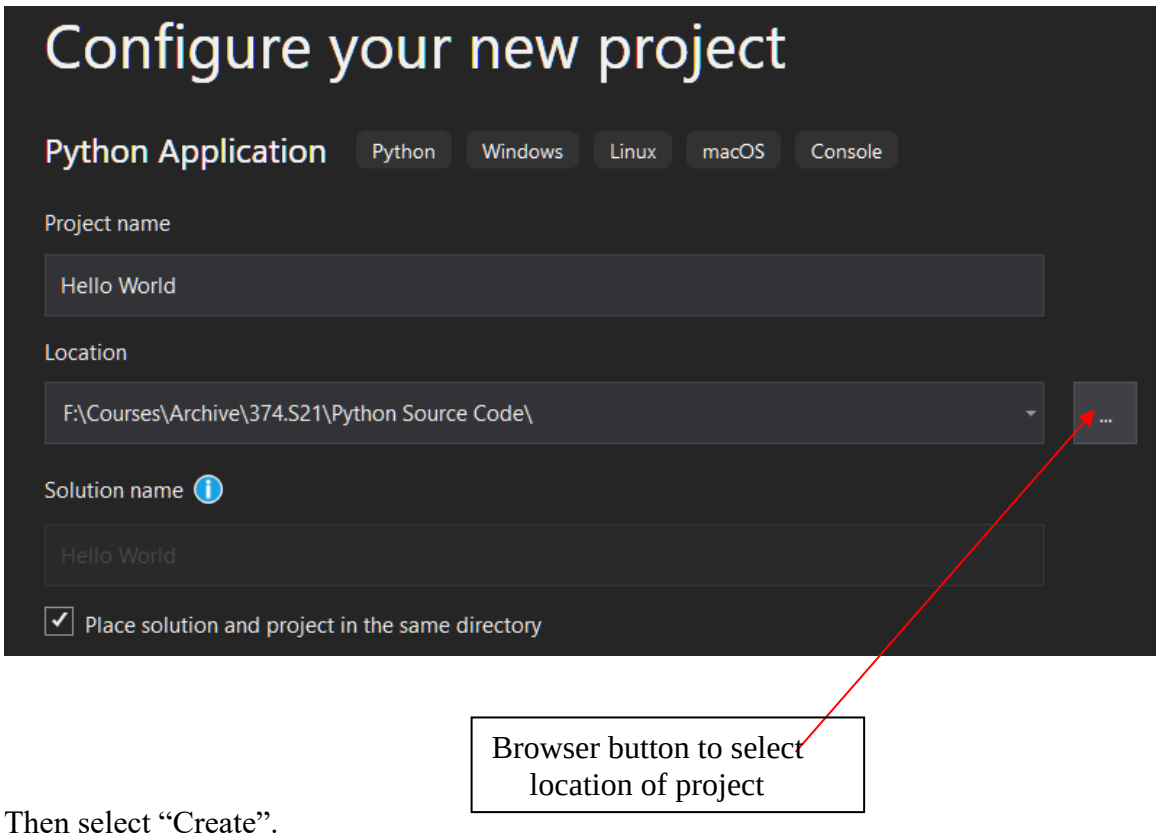
lower half), find the row with “Path” in the first column, and click “Edit…”, (5) click “New” and type (or copy and paste) the new path. For instance, it should look similar to:

C:\Users\UserName\AppData\Roaming\Python\Python*xx*\Scripts

depending upon what your “username” is (*xx* is the version number of your Python programming language). You can always find out which directories are in your PATH by typing: `$env:PATH` in your PowerShell window.

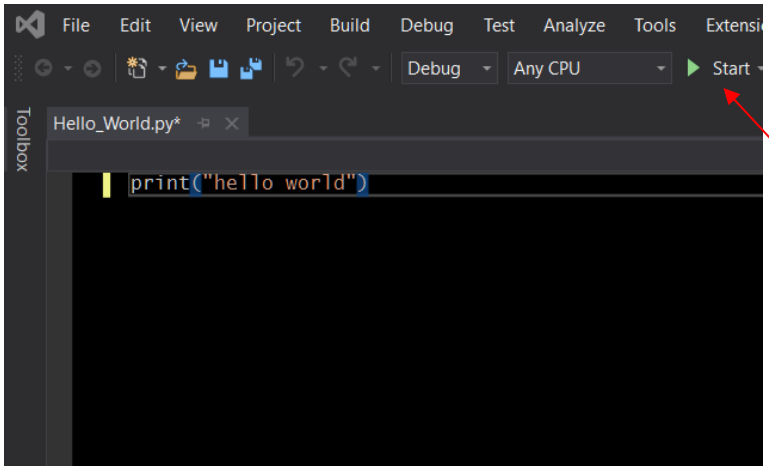
Writing Code in Python

Now that Python has been installed, we can now start writing Python code. Start the Microsoft Visual Studio application and click “continue without code”. Click on “File” → “New” → “Project…”. Under “All languages” select “Python”. Then select the “Python Application” row, and then select “Next”. Name the “Project name” as “Hello World”. Select the “Browse” button to put the project in a directory of your own choosing.

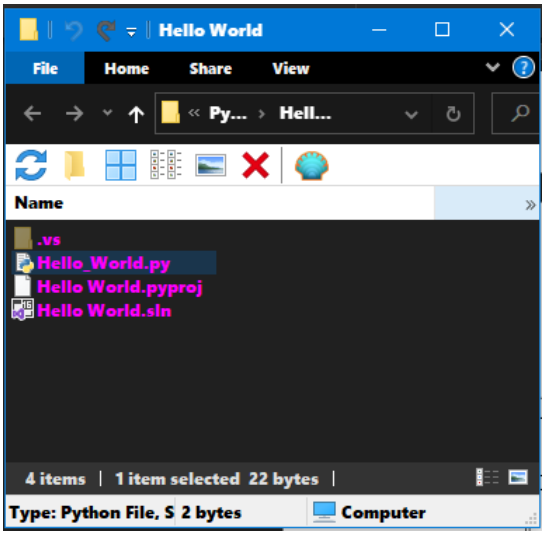


Then select “Create”.

In the *Hello_World.py* window, type: `print("hello world")`



Click on the "Start" button (green arrow triangle), and a console window should appear with the phrase "hello world". You have now written your 1st Python application. If you go to the folder where your Python code lies, you should see the following:



The *.py file is the source code, the *.sln file is the Solution file (containing the project). Double clicking on the Solution file opens the Python project.

Writing Python GUI with Tcl/Tk

The previous section showed how to write code for command line applications that rely on a console for operation. In this section we will write code that uses the window environment of Windows, Mac, and Linux operating systems. Thus, we will write a windows-driven rather than a command-line driven program using the widgets available in the Tcl/Tk package called *tkinter*. There is a good tutorial on the web located at:

https://learn.sparkfun.com/tutorials/python-gui-guide-introduction-to-tkinter/hello-world

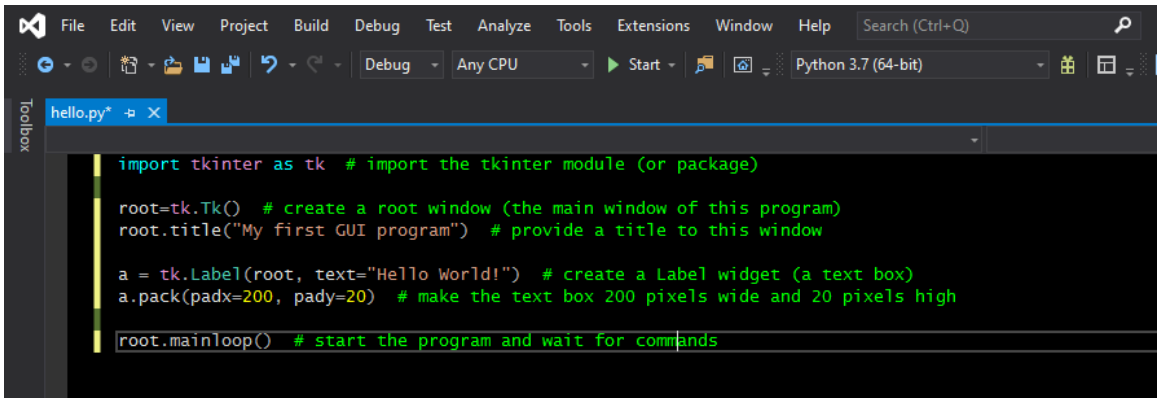
Read Shawn Hymel's tutorial called "Python GUI Guide: Introduction to Tkinter" on the webpage above. The code below is based on his tutorial. Create a new Python program called *Hello.py*, and copy and paste the code below and run it:

```
import tkinter as tk  # import the tkinter module (or package)

root=tk.Tk()  # create a root window (the main window of this program)
root.title("My first GUI program")  # provide a title to this window

a = tk.Label(root, text="Hello World!")  # create a Label widget (a text box)
a.pack(padx=200, pady=20)  # make the text box 200 pixels wide and 20 pixels high

root.mainloop()  # start the program and wait for commands
```



Upload to Blackboard your source code (*.py) of your Python programs *Hello_World* and *Hello*. You will see an assignment on Blackboard called **Python Tutorial #1**.