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SPREADSHEET APPLICATIONS IN CHEMISTRY USING MICROSOFT® EXCEL®

DATA PROCESSING AND VISUALIZATION

SECOND EDITION

with website

WILEY

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Chapter 6

Spreadsheet Applications in Chemistry Using Microsoft® Excel®

Data Processing and Visualization

Second Edition

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Preface

Since the publication of the first edition of this book almost 25 years ago, there have been monumental changes in how we interact with experimental data as scientists. We can now store it more securely, visualize it in new ways, share and collaborate on it, and more deeply interpret it, thanks to new and constantly improving data processing tools coming on stream. The spreadsheet today as a data processing tool is very accessible and can visualize calculations and help make theory and experimental data come to life so that it is meaningful to the student. This new edition of the book retains its guided tutorial approach for teaching undergraduate and postgraduate students a range of chemistry topics that incorporate aspects of data analysis and also provide for visualizations of fundamental concepts.

In this edition, we have included additional datasets along with guided tutorials for the student to work through independently. The datasets and guided tutorials are designed around Excel but, if Excel is not available, the exercises can also be navigated in other spreadsheet programmes, e.g. Google Spreadsheets or LibreOffice Calc. Similar functionalities are available across all these programmes.

We have expanded the content on some important topics such as *statistical treatment of data* and *calibration in analytical chemistry,* for example, that were not included in the previous edition. The book brings the student from the basics of navigating a spreadsheet for simple data processing operations in a step-by-step manner, to advanced data processing and analysis for small and medium-sized datasets. The chapters are intended to give students practical experience in performing spreadsheet calculations and visualizing experimental results. There is an emphasis on letting the learner gain enough familiarity and experience to enable them use spreadsheets independently, and in other scientific contexts, while at the same time encouraging the student to examine data objectively and critically interpret it as an experimental scientist. This book provides an experiential ‘learn by doing’ approach to gain conceptual insights as well as practical expertise in data analysis in chemistry topics.

Acknowledgements

This book is the culmination of many combined years of teaching and research experience for us both. We would like to thank our families who travelled the journal of this book writing venture, from the initial blank page and the pontificating, to the reading and suggestions to improve the offering, to the proofing of the final manuscript. It was a long road, but would have been infinitely longer without you. In particular, Aoife would like to thank David for his infinite support during the burning of midnight oil to get the chapters inked, and Ciara for putting time into shaping and structuring the content with her vision; and Dermot would like to thank Tara for her never-ending patience with him.

We have also leaned on our colleagues in Dublin City University who have kindly supplied us with experimental datasets to use in one or both editions of this book: Francisco Saez, Robert Forster, Brendan O'Connor, Ciarán Fagan, Conor Long, Han Vos, Tia Keyes, Blánaid White, and Fiona Regan. The book would not be as rich without your input. Thank you.

Navigation of the Book

There are six concise chapters in this book that take the learner from basic spreadsheet navigation to complex data analysis approaches reasonably quickly. The book is designed to start at the basics so that no prior experience of spreadsheets or Excel is required. The book is not intended to be passively read, but instead to be actively used while sitting in front of a computer. Each chapter sets out its own learning objectives and is divided into sub-sections that are focussed on covering basic theory needed to understand the scientific concepts and datasets in the accompanying guided tutorials. Additional questions are given at the end of each chapter to push the student in applying spreadsheet procedures in other scientific contexts.

About the Companion Website

This book is accompanied by a companion website.

www.wiley.com/go/morrin/spreadsheetchemistry2

This website includes:

Students' resources

- Worksheets
- Further Exercises

Teachers' resources

- Worksheets
- Further Exercises

1
Introduction to Excel

In this chapter, students will learn to:

- Undertake basic operations in an Excel worksheet
- Perform mathematical calculations on worksheet data using formulas and functions
- Understand and apply relative and absolute cell referencing
- Visualize and interpret data sets in the form of charts

Excel is a Microsoft spreadsheet application widely used to store, organize, process and analyze many forms of data, including experimental data. It offers great flexibility and is, in many respects, unrivalled in terms of its functions as applicable to scientific experimental data. Researchers use spreadsheet applications such as Excel to work with experimental data. For example, they will transfer data to a spreadsheet such as Excel to:

- Store and organize experimental data
- Manipulate data using mathematical functions
- Visualize data, for example, through charts and tables
- Perform statistical analysis of data
- Apply curve fitting with linear and non-linear regression

Besides Excel, other examples of spreadsheet applications exist including free, open source software packages such as LibreOffice Calc and Google Spreadsheets. They operate in a similar manner to Excel in general, but differ in some features and hence functionality. Microsoft® Excel® has the most features and is currently more widely used than these open source alternatives. That said, the landscape is rapidly changing and these open source software packages are increasing in maturity and popularity. If you have access to Excel, it is the spreadsheet software program of choice. As such, the tutorials in this book are designed specifically around Excel. However, if Excel is not accessible, open source alternatives are a good option to work through the tutorials to learn approaches to processing experimental data.

This chapter introduces basic standard worksheet operations in Excel that will be needed for the later chapters. The tutorial exercises have been designed around Excel for PC. If you are using Excel for Mac, you can expect minor deviations from the tutorial instructions, as formats and styles, and locations of commands and options can differ between the two versions. Likewise, accessing tools and commands may differ if you are using an early version of Excel. However, most functionality is equivalent between versions and so all tutorials here can be undertaken using any version of Excel. Of course, it is advisable to upgrade Office if you are using a particularly archaic version. Once you are up and running with Excel, it is worth spending time working through the tutorials in this chapter to ensure that the more basic spreadsheet functions of Excel are understood before moving to the more advanced topics and tutorials in later chapters.

1.1 Navigating the Workbook

1.1.1 The Worksheet

Launching Excel brings you into a workbook containing a set of spreadsheets. Excel refers to each spreadsheet within a workbook as a ‘worksheet’. Some basic aspects of the worksheet are labelled in Figure 1.1.

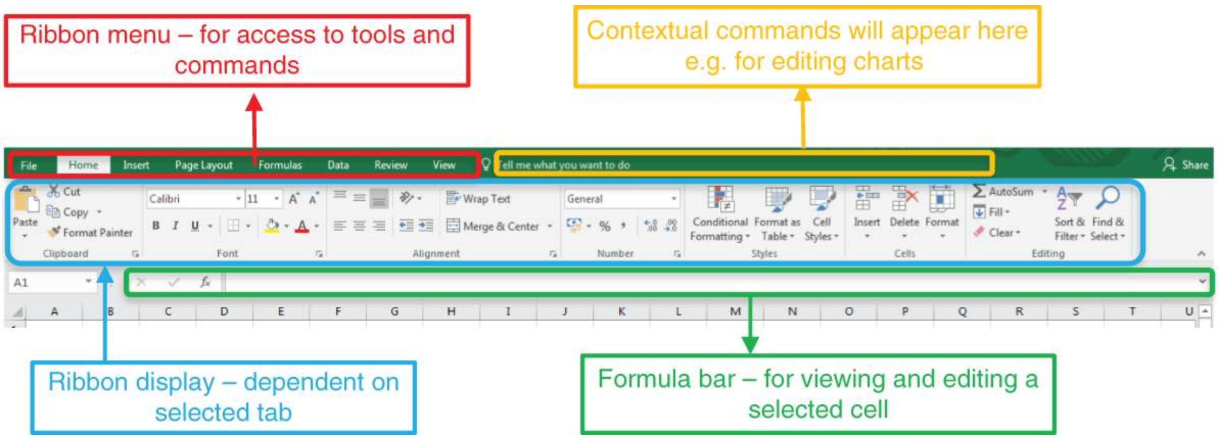


Figure 1.1 Highlighted aspects of Excel worksheet for navigation.

The **Ribbon menu** gives access to all tools and commands. Within the Ribbon tab, you can see several tabs – Home, Insert, Page Layout, Formula, Data, Review, and View. Each of these has their own **Ribbon display**, which comprises groups of buttons representing a variety of commands that are displayed when each tab is selected.

Contextual tabs are special types of tabs that appear only when an object is selected, such as a chart or a shape. These contextual tabs contain commands specific to whatever object you are currently working on. For example, after you add a shape to a worksheet, a new **Format** tab appears as a **Contextual tab**. These tabs only activate when you work with particular objects. You will use these tabs regularly in the tutorials in this book.

The **Formula bar** is the toolbar at the top of the worksheet window that can be used to enter or copy an existing formula into cells. It is labelled with the function symbol *fx*.

By clicking the **Formula bar**, or when you type the equal (=) symbol in a cell, the **Formula bar** will activate.

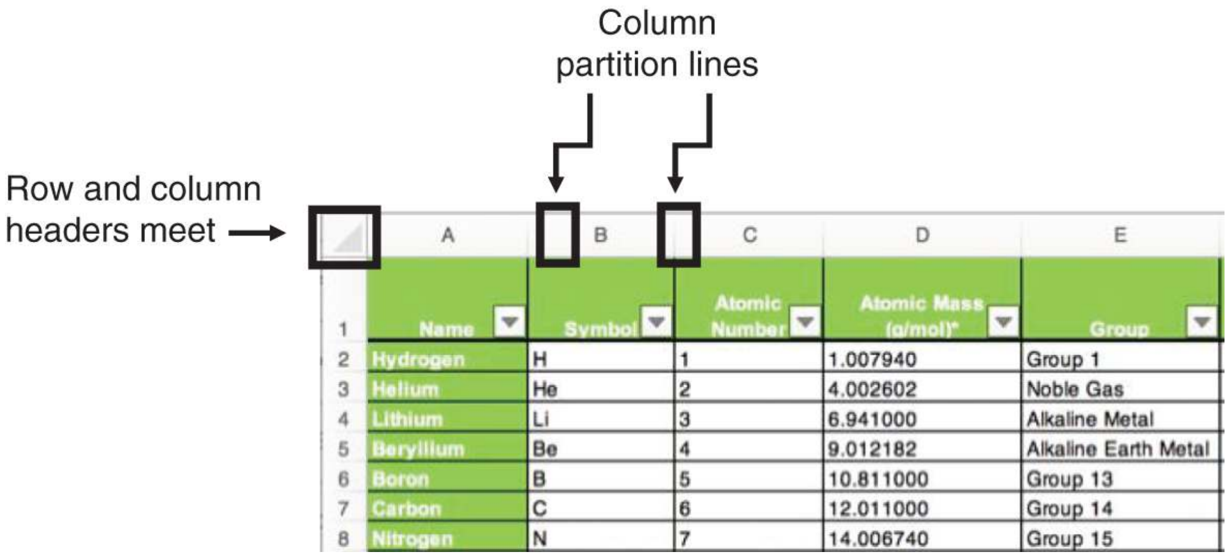
1.1.2 Worksheet Tools

You can navigate the Excel worksheet fairly intuitively using standard Office365 operations. The first tutorial here will use an already populated worksheet to show you some of the tools available.

Tutorial 1.1 Using Basic Formatting and Analysis Commands

In this tutorial, you will work with a data set relating to the Periodic Table to learn some basic formatting and analysis commands in Excel.

- Open the workbook *1.1_Periodic Table.xls*.
- In the worksheet, you will see columns of data related to the periodic table. Expand the width of the columns so that all text in each of the columns can be seen. To do this, bring the mouse cursor to where the row and column headers meet – see Figure 1.2. By clicking here you will select the whole worksheet. Then double-click any one of the column partition lines. This will readjust all column widths so that you can visualize the data clearly.



	A	B	C	D	E
1	Name	Symbol	Atomic Number	Atomic Mass (g/mol)*	Group
2	Hydrogen	H	1	1.007940	Group 1
3	Helium	He	2	4.002602	Noble Gas
4	Lithium	Li	3	6.941000	Alkaline Metal
5	Beryllium	Be	4	9.012182	Alkaline Earth Metal
6	Boron	B	5	10.811000	Group 13
7	Carbon	C	6	12.011000	Group 14
8	Nitrogen	N	7	14.006740	Group 15

Figure 1.2 Periodic table worksheet highlighting row and column formatting navigation.

- Now take a look at column D – *Atomic Mass*. The values in the cells have 7 decimal places reported which is unnecessary for our purposes. To reduce the number of significant figures, first highlight the data by clicking at the top of column D. Right click and select **Format Cells**. In the pop-up dialogue box, select **Number** and enter *3* in the **Decimal Places** box. Press **OK**.
- Next, format the columns of data into a table so that you can sort the data. Highlight columns A to I and under the **Home** tab, click **Format as Table**. Choose a style you like in the dialogue box that pops up. Ensure **Header Row** is ticked in the **Table Style Options** under the contextual **Design** tab.
- Next, sort the data in increasing order of atomic radius.

  Select the greyed icon  in G1 to the right of text *Atomic Radius*. Click on **Smallest to Largest** and exit out of the box.

○ Also try sorting the data indifferent ways according to the different properties listed.

- You can visualize the data by creating charts to represent the data. Try graphing *Atomic Number* against *Atomic Mass*. To do this, highlight columns C and D. Click the **Insert** tab and then click **Scatter** chart type as shown in Figure 1.3. This type of chart is very common when working with experimental data.

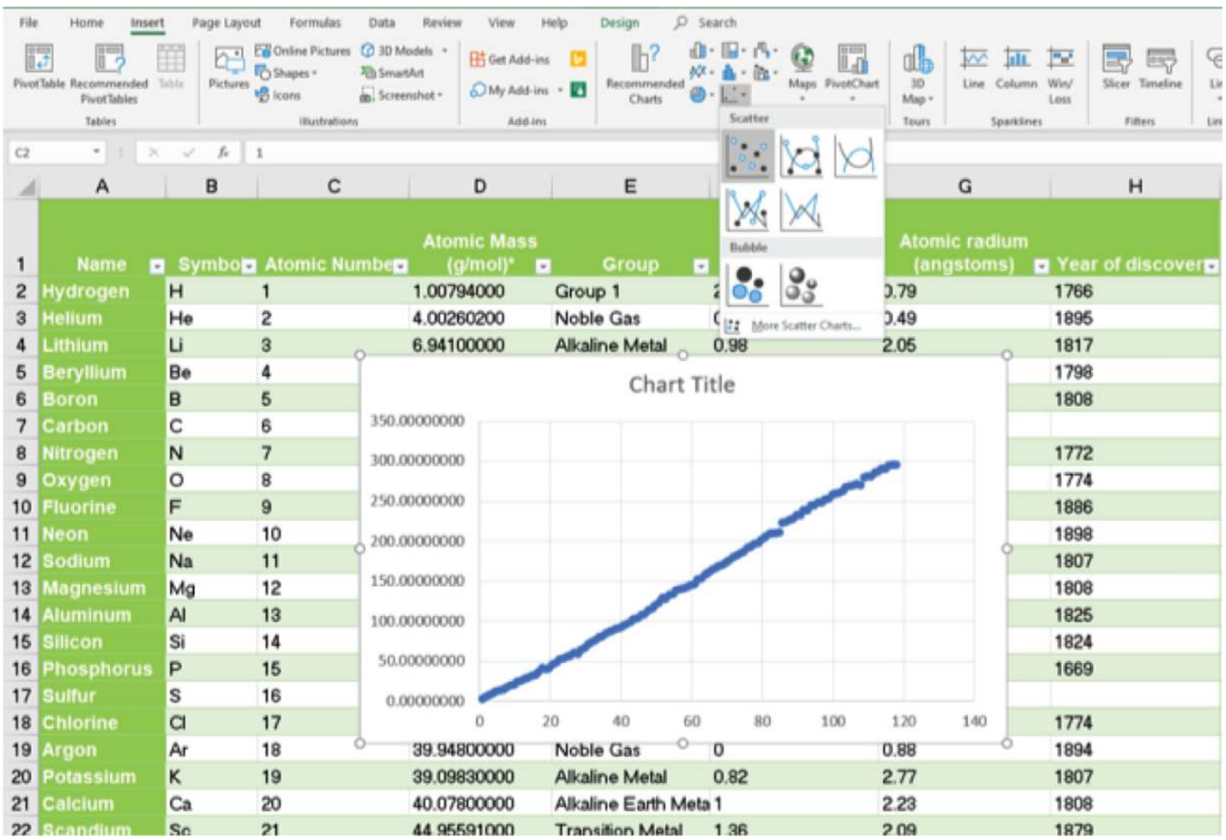


Figure 1.3 Generating a scatterplot in an Excel worksheet.

- To format the chart, select the chart and double click into each **axis title** and **chart title** to edit the text.

- Click on the *x*-axis, and right click and select the **Format Axis** option. Select **Tick Marks** and in the **Major Type** box, and select **Inside** to add tick marks to the *x*-axis. Repeat this for the *y*-axis.

- **Gridlines** are the light grey horizontal and perpendicular lines that divide the chart area into squares to form a grid. To delete these, click on one of the horizontal gridlines, and then right click and select **Delete**. Repeat this step for the vertical gridlines.
- Click through the previews in the **chart styles** to change the layout or style to one you like. Depending on your chosen style, your chart might look something like in Figure 1.4.

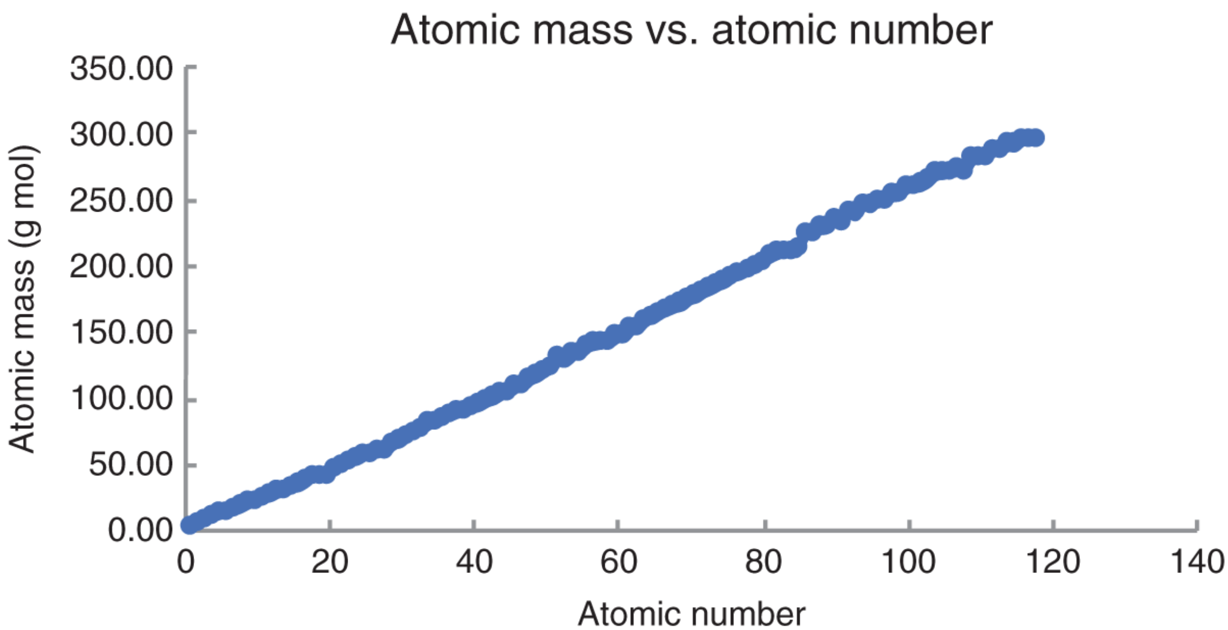


Figure 1.4 Formatted chart showing the linear relationship between atomic mass and atomic number.

- Using the same approach, create charts to visualize the dependence of electronegativity and atomic radius on atomic number. Decide yourself on the chart type and format and design that you use.
- Save and close the *1.1_Periodic Table.xls* workbook.

1.2 Mathematical Operations on Cells

1.2.1 Formulas and Functions

Once data is entered into a worksheet, operations can be performed to process the data. Excel performs mathematical operations using formulas and functions. Formulas can be written into the formula bar and always begin with an equals sign (=).

These formulas and functions act on specified cells in a worksheet, where variables can be defined in other cells that are referenced. There are two types of cell references used by Excel: relative and absolute. Relative and absolute behave differently when copied and filled from other cells. Using a letter-number combination, e.g. A2, to describe a cell is known as relative referencing. By default, all cell references are relative references. These references change based on position relative to the original cell when the formula is copied and pasted into another cell. The effect is to keep the relative addresses between cells referenced in a formula, in effect making these variables.

In contrast, absolute referencing uses the format $letter$number, e.g. A2, and remains constant when copied and filled from other cells. If the absolute reference A2 had been used as the address, then this address is maintained in the formula across all cells, effectively rendering it a constant (the value of the number in cell A2).

The following tutorials have examples of using both relative and absolute referencing.