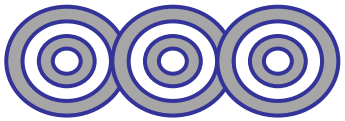
Computer Applications in Chemistry



An overview of the applications of computers in chemistry

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Applications of Computers

Computer plays a very important role in every aspects of our lives, including chemistry.

Applications of Computers in Chemistry

Two types of applications:

- **Interfacing:**

A computer is connected to an instrument for data collection and control the system.

- **Software applications:**

Data analysis, simulation, structural searching, modelling, drug design, etc.

General Features of Computer

- Able to perform operations very fast.
- Very low error rate.
- Ability to process various types of information – not only numerical quantities.
- Ability to store programs and data.

Fields of Application

- Computational Chemistry
- Chemometrics
- Chemoinformatics

Computational Chemistry

• A branch of chemistry that uses the results of theoretical chemistry incorporated into efficient computer programs to calculate the structures and properties of molecules and solids, applying these programs to real chemical problems.

• **Computational Chemistry** – when a mathematical method is well developed and can be implemented on a computer.

• **Examples:**
-Quantum mechanics,
-Molecular mechanics,
-Simulation,
-Modelling,
-Minimisation,
-Conformational analysis.

Chemometrics

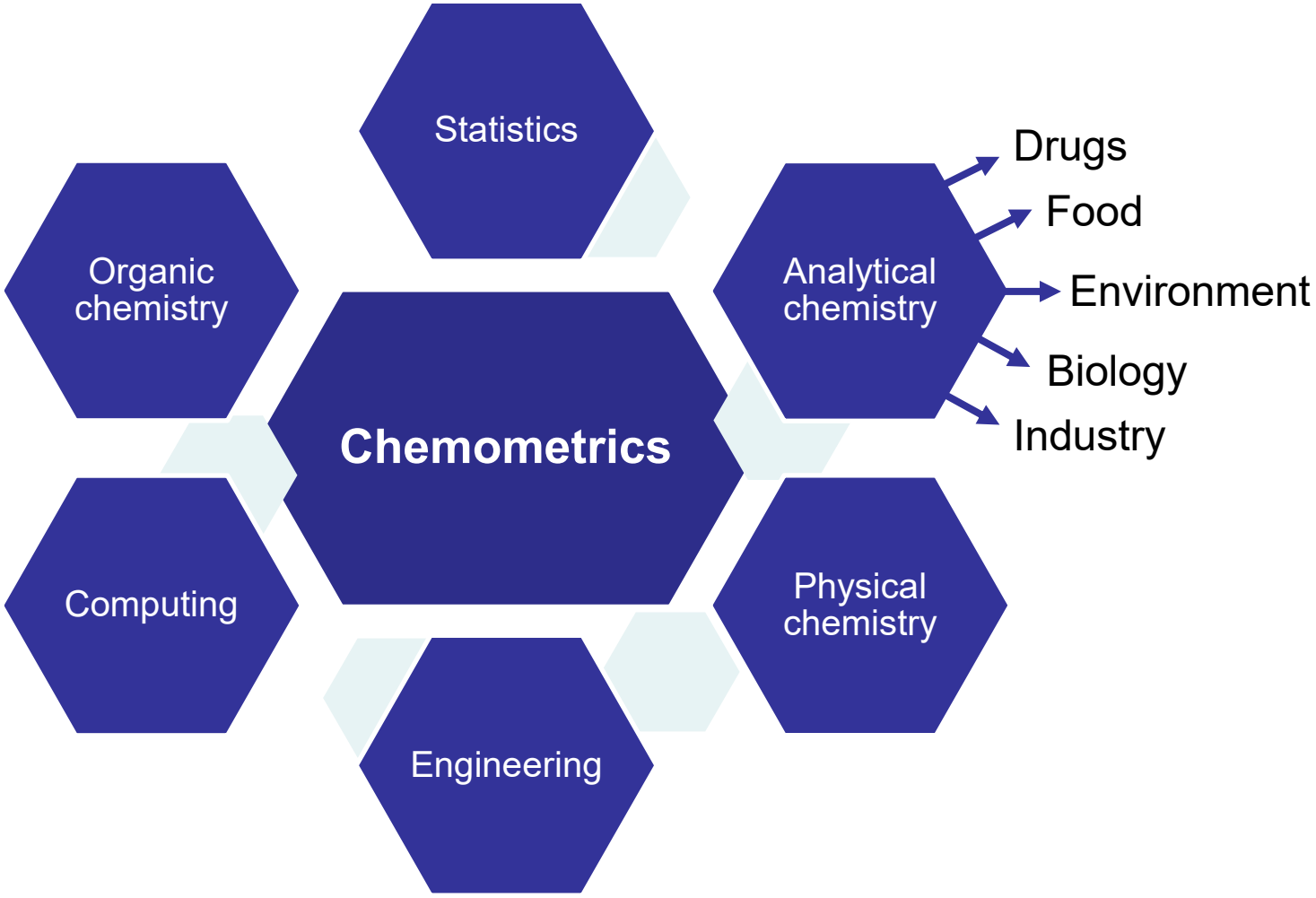
- The science of relating measurements made on a chemical system or process to the state of the system via application of mathematical or statistical methods.

- The chemical discipline that uses mathematical and statistical methods to design or select optimal measurement procedures and experiments, and to provide maximum relevant chemical information by analyzing chemical data.

- **Examples:**

-Experimental design,
-Calibration,
-Signal processing,
-Pattern recognition.

Chemometrics and other disciplines



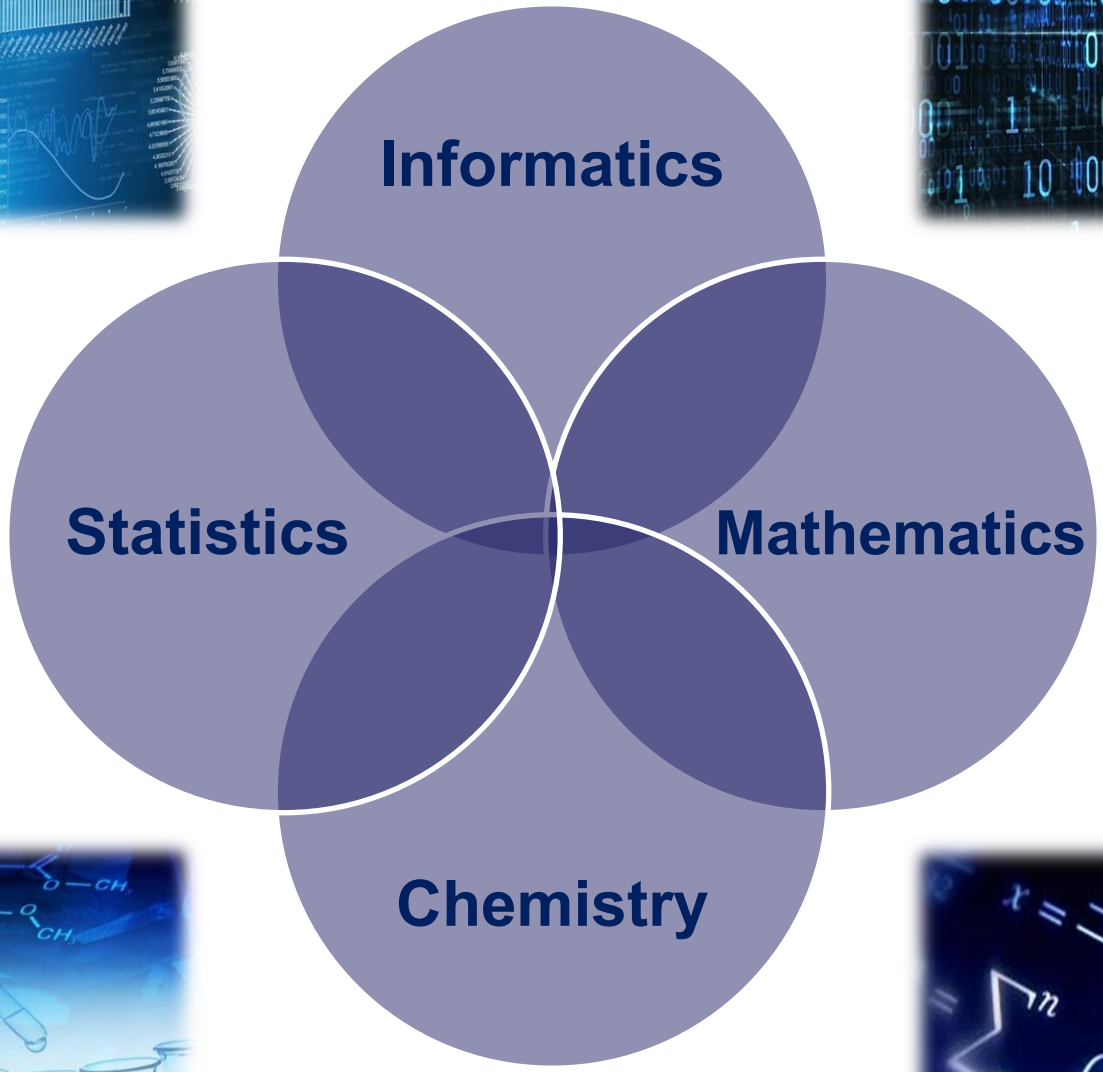
Chemoinformatics

- The application of informatics methods to solve chemical problems.

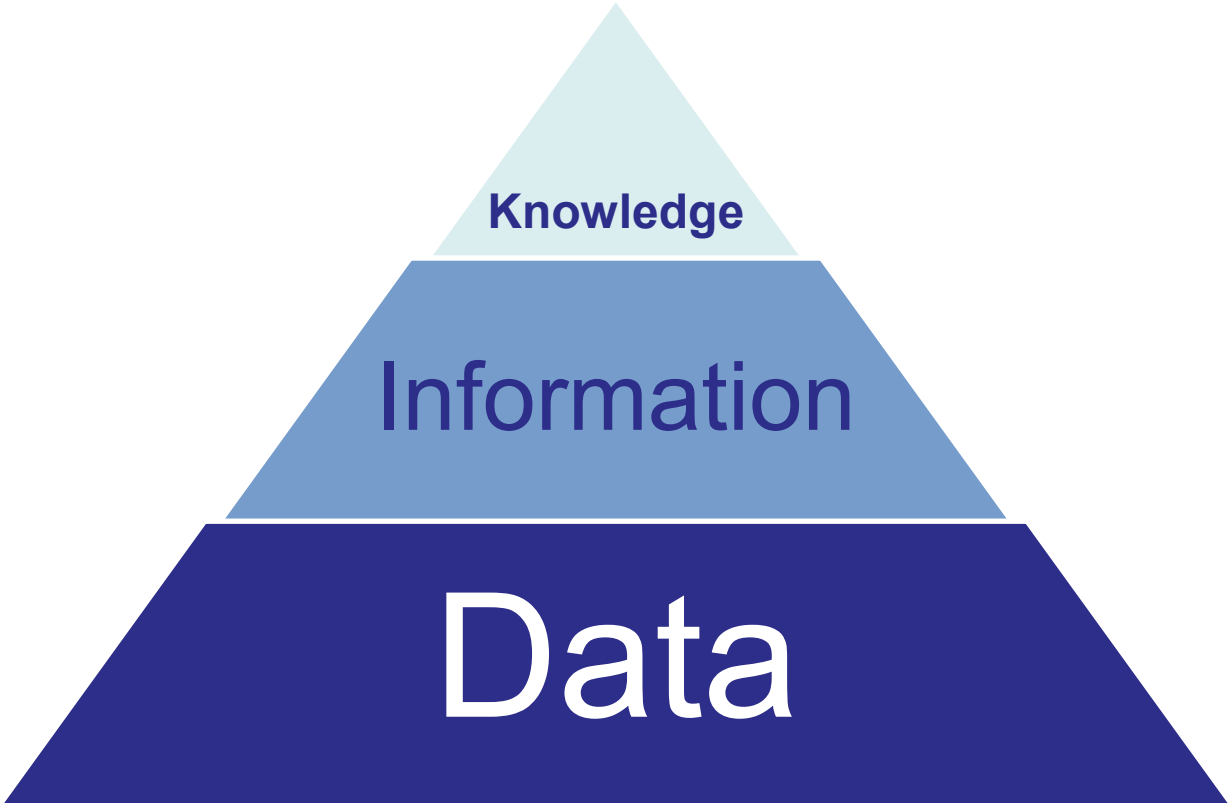
- The application of informatics to the management and processing of data, information and knowledge in chemistry.

- **Examples:**

-Storage and searching of chemical structures,
-Quantitative Structure-Activity Relationships (QSAR),
-Structure elucidation,
-Drug design.


Informatics
Statistics
Mathematics
Chemistry

From Data to Knowledge



Abstraction

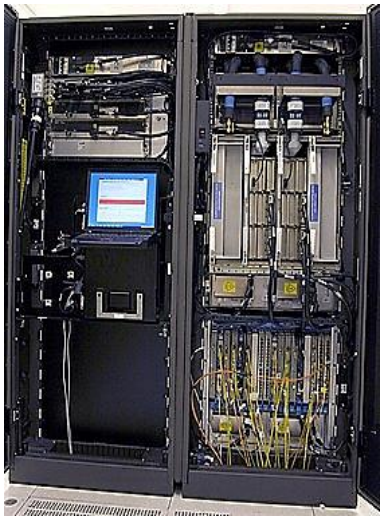
Context

Measurements
Calculations

Types of Computer

Classes by purpose

-Microcomputers (personal computers)
-Minicomputers (mid-range computers)
-Mainframe computers
-Supercomputers



Classes by function

-Servers
-Workstations
-Information appliances
-Embedded computers

Classes by usage

-Public computer
-Personal computer
-Shared computer
-Display computer

Classes by generation of technology

-1st generation computers (1940-1955): Vacuum Tubes
-2nd generation computers (1956-1963): Discrete Transistors
-3rd generation computers (1964-1970): Integrated Circuits (ICs)
-4th generation computers(1971-present): Microprocessors

Operating Systems

Windows

- Operating system based on graphical user interface GUI on PC.
- Windows 95, Win 98, Win 2000, Windows XP, Vista, Windows 7, Windows 10.

Unix

- A multiuser, multi-tasking operating system.
- Developed in Bell Labs in early 1970s.
- Used in workstations, e.g., Solaris, AIX.
- Can also be used in PC.

Linux

- Free UNIX.
- Originally developed by Linus Torvalds, 1991.
- Red Hat, Fedora, Slackware, Debian, Ubuntu.

Mac-OS

- Operating system on a macintosh.
- Easy to use, very user friendly.

Programming Languages

Allows a user to communicate (give instructions) to the computer

A person who wants to develop a computer application must know at least one programming language.

Example programming languages:
BASIC, Visual Basic, Fortran, Pascal, C, C#, C++, Java, PHP, Python.

Chemistry in Computers

Basically, chemistry and chemical compounds and elements are used in **hardware.**

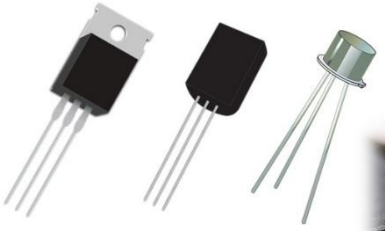
CRT

LCD

LED

Monitors

Chips



Transistors

Solder

Batteries

Cables

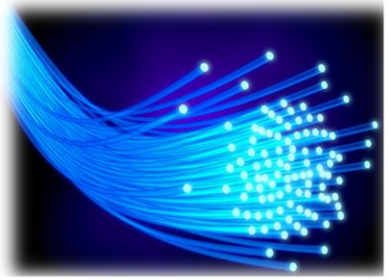
Insulating sheets

Capacitors

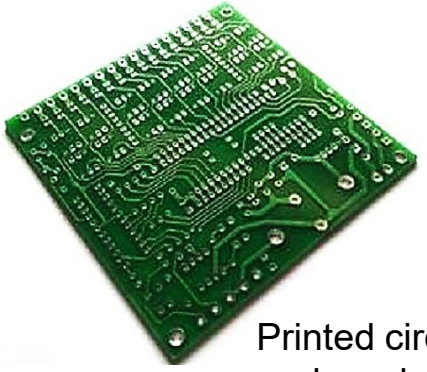
Integrated circuits (IC)

Cases

Light-emitting diodes (LED)



Optical fibers



Printed circuit boards

Resistors


Thank You!