CCDC
advancing structural science

Identikit.

Directions for activity leaders

In this handout you will find guidelines for the activity leaders (parents, teachers, responsible adults) to guide the detectives (learners) in the activity "Identikit of Common Substances".
This handout consists of two parts:

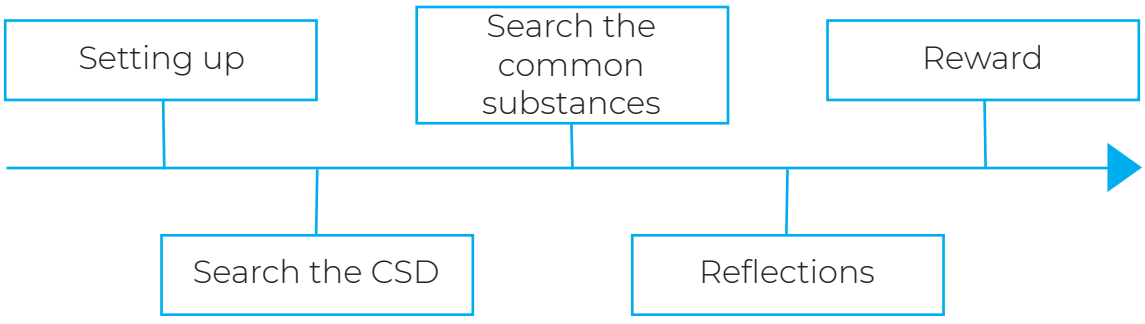
1. **Directions** for setting up and leading the activity
2. Ideas to support the **guided reflection** when discussing the findings at the end of the research. These include a **glossary** to support the detectives throughout the activity. Reflections and glossary can be found from page 5 onwards.

Tip: Search for the words in **bold** in the glossary at the end of this document.

Before starting: This activity is carried out at your own risk. Please read the health and safety guidelines on our **webpage** to reduce risks.

Guide to the activity

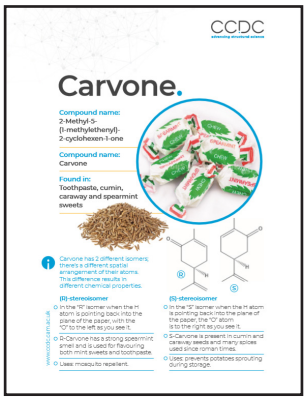
This activity will take approximately from 30 minutes to a couple of hours, depending on how you decide to deliver the activity.



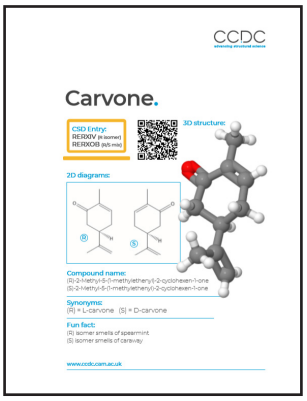
Setting up

1 Collect the common substances material listed in the "What you will need" section on the webpage and prepare the common substances handouts.

The *common substances handouts* provide more information about the substances investigated and are designed to be used with the identikit worksheet. They are in two parts:



Page 1: A handout for the detective (the learner) to find out more about the substance.



Page 2: An answer sheet for the activity leader to guide the learners in filling in the identikits.

In setting up the activity you can be as creative as you like! You can, for example, have all the materials and handouts (pages 1) displayed on one table, and the **detectives** will come to it to fill in their identikits. Or you can decide to organise a treasure hunt, so that the detectives will need to look for the materials and handouts around the space you decide to dedicate to the activity.

If you do not have the opportunity to print out the handouts or collect all or part of the material, do not worry: you can still carry out this activity online.

2 Provide each detective with one or more identikit sheets. This is the document ***Activity Worksheet - Identikit***. Each identikit sheet will contain the information for one structure, i.e., associated with one **refcode**.

If you cannot or do not wish to print, you can reproduce the identikit page on a piece of paper.

Start the activity - Search the CSD

3 This activity can be carried out either individually or in teams, as it suits your situation better (number of detectives, adults supervising). For example, the entire team can research one substance at a time working together, taking lead on different roles each time. Otherwise, different team members may investigate different structures and then report back their findings to discuss with the team. An option between these two could be creating smaller sub-teams.

To start, show the **refcode** lists to the detectives (page 1 of document ***Pick a refcode and search the CSD***), from which they will pick the structure to investigate. The refcode chosen is to be written in the **STEP 1** field of the identikit.

STEP 1 Pick a refcode and write it down.

CITRAC10

4 Search the **CSD** for the structure associated with the refcode chosen.

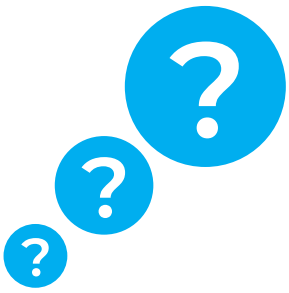
To search the CSD you can:

1. Scan the QR codes provided using a smartphone.
2. Insert the refcode in the Access Structures portal on the CCDC website at this **link**.

Both ways are presented in detail in pages 2 and 3 of the handout *Pick a refcode and search the CSD*. To facilitate this step, direct links to each structure page are also available via clicking the links in the "Find out more" section in the activity webpage.

For the Home Learning activity, you can ignore pages 4 and 5 of the handout, which show instead other ways for licensed users of the CSDSystem to search the CSD. These are **NOT** required **NOR** necessary for this activity, which can be completed without a license. However, if you are already an avid user of the CSD and want to help your detectives to use these tools then pages 4 and 5 will help you on that journey.

The method employed for searching the CSD (QR code or Access Structures) should be inserted in **STEP 2** of the identikit.



5 Each **crystal** structure's webpage will provide the detective the information to fill fields in the identikit from **STEP 3** to **STEP 5** .

To support drawing the molecules, the 3D representation on the website uses the following colours: grey for carbon atoms, red for oxygen atoms and white for hydrogen atoms. The *common substances handouts* also include this representation.

Search the common substances

6 The hunt shall begin! With the information from the identikit, the detectives can now search for the common substance that corresponds to the crystal structure they chose, via reading the substances handouts and comparing the information therein with their identikit. This part of the activity will be shaped based on the solution you chose for the set up.

This will allow the detectives to fill in **STEP 6** of the identikit!

Discussion and Reward

7 When all (or some of) the structures have been found and their identikits filled in, we recommend discussing the findings with the detectives. Some points of discussion and a glossary are suggested in the following pages. You can refer to the glossary at any time during the activity to help the detectives filling in their identikits.

8 It is now time for the detectives to collect their reward badge! You can download the collectable virtual badge following the instructions on our webpage.

Guided discussion

The guided discussion explores some questions that you could ask the detectives when they have completed the activity.

To begin with, analyse which elements are in each of the molecules found and compare. How many elements do you identify?

The **molecules** that are present in our common substances are composed from the same three (only 3!) elements: **C**, **H**, **O**. To deepen this insight from the activity, you can visit the **periodic table of crystals** on our website, where you can see how frequently each element is found in our database, the CSD. How frequent are the three elements we found in this activity? You will find that C, H, and O are the most abundant elements in the CSD.

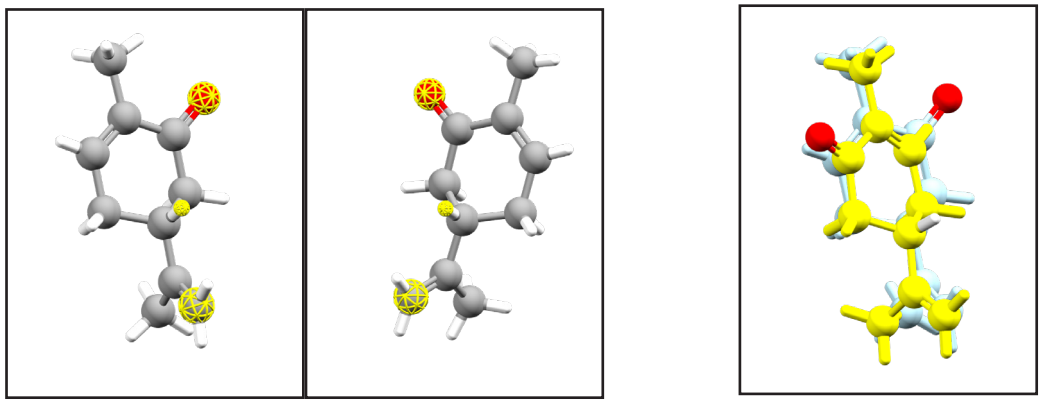
Do you know any other molecules? Which elements appear in such molecules?

3 elements, 7 molecules. Reflect on how different the properties of the common substances are. Where do these differences come from?

Using the diagrams of the molecules that the detectives drew, or the common substances handouts, or the webpages of the structures, guide the detectives to observe the **bonds** that the **atoms** form with each other, and the geometry that such bonds create for the molecules.

Just three atoms can make up so many molecules with completely different properties!

To further reflect on this point, observe the two molecules of carvone. As the detectives found on the handout, there are two **stereoisomers**. This means that the molecules of each isomers have the same connectivity (i.e., same **formula**, same atoms, and same bonds), but in 3D you cannot completely overlap stereoisomers with any rotation. Observe the panels in the following page.



Panel 1: (R)-stereoisomer of carvone (from structure with refcode **RERXIV**).
Panel 2: (S)-stereoisomer of carvone (from structure with refcode **KOSNIS**).
Carbon atoms are in grey, oxygen in red, and hydrogen in white. In panels 1 and 2 three atoms are highlighted to help observe the difference.
Panel 3: the (S)-stereoisomer (yellow) is rotated and tentatively overlapped to the (R)-stereoisomer (light blue). This shows that it is not possible to completely overlap the two stereoisomers.

A typical example to explain isomers are your hands: they look the same, but if you stuck them on top of each other, you cannot rotate them in any way to obtain a perfect overlap!

Stereoisomers might present different properties, as the description of carvone shows. The 3D geometry of the molecule is very important to determine the properties of the compound.

If you are curious to see how the 3D organisation of molecules in crystal structures effects the properties of the crystal, do not miss the **Lego, Chocolate and Polymorphs activity**!

As additional reflections, you can also invite the detectives to think about which other materials they know that might contain the molecules investigated, or which substances might contain a crystal structure.

Glossary

Atoms are the basic building-block of all matter and are the smallest unit of a chemical element. Did you know the word atom comes from Greek and means "*that cannot be cut*"?

Bonds are strong chemical connections formed between atoms.

A **molecule** is a group of two or more atoms that are held together by bonds.

A **crystal** is a solid material where molecules or atoms are packed in an ordered way. Crystals have specific geometries and shapes.

The **formula** of a compound is a list of all the elements present in the molecule. Each element is followed by a subscript number to specify how many atoms of that element are present.
As an example, in a water molecule there are two hydrogen atoms (H) and one oxygen (O): its formula is thus H_2O.

Stereoisomers are molecules that have the same formula and same connectivity of the atoms, but their 3D geometry is different so that they cannot be completely overlapped.

CSD is the acronym for Cambridge Structural Database. This is the database curated by the CCDC that contains the data of over 1 million crystal structures!

Refcode is the identifier given to each crystal structure present in the CSD. This is composed by a sequence of six letters and, in some cases, two numbers. The refcode is unique to each structure and will help you to find one structure in a million.

The **detectives** (or CSD Detectives) are our new generation of scientists on a quest to discover more about common substances and crystals. If you have some of the substances like mints and chocolates, don't be surprised if your eager detective also wants to experience the taste of the substance!