Sunscreen structures

Education in Chemistry
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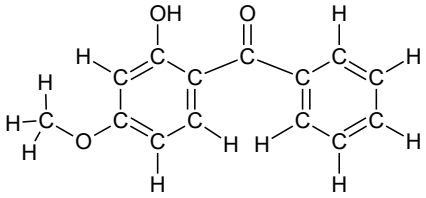
Certain functional groups play an important role in providing sunscreen chemicals with their UV-absorbing properties. Read the article on reef-friendly sunscreens and answer the questions below.

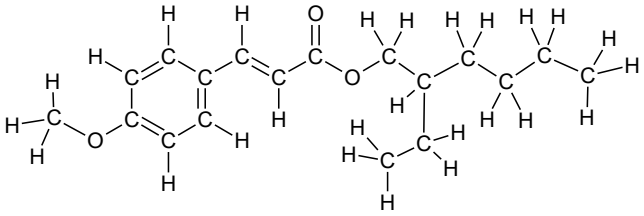
1. On 1 January 2020, the Pacific Island of Palau will become the first country to ban all sunscreens that contain any one of 10 chemicals.

   The structure and names of three of these banned chemicals are shown in **Figure 1**.

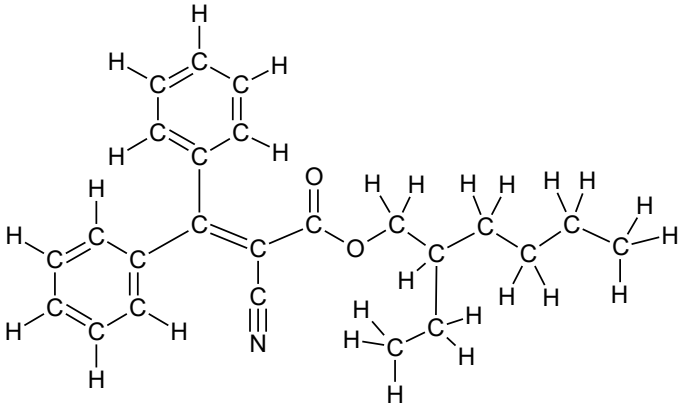
Figure 1



oxybenzone



octinoxate



octocrylene

   a. Highlight the following functional groups on the structures given in **Figure 1**;

      i. alkene

      ii. alcohol

      iii. ester

   b. All of the molecules in **Figure 1** have UV protecting properties.

      Their ability to absorb UV radiation is based on their structure.

      Look at the structures of the molecules.

      i. How are the structures of oxybenzone and octinoxate similar?

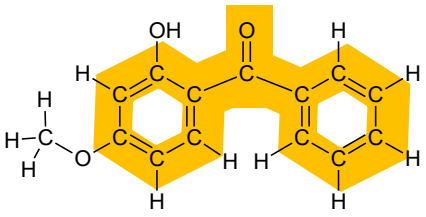
      ii. How are the structures of octinoxate and octocrylene similar?

c. The molecules in **Figure 1** are all able to absorb UV radiation because they contain a conjugated system.

A conjugated system is when every other bond is a double (=) or triple (≡) bond. The double/triple bond can be between two carbon atoms, or a carbon atom and any other type of atom.

The conjugated system in oxybenzone is highlighted in **Figure 2** below.

Figure 2



Highlight the conjugated system in octinoxate and octocryolene on the diagrams in **Figure 1**.

Extension: Dutch researchers have developed a new form of sunscreen in which natural UV protectants are encapsulated in a coating of natural polymers.

Find out the structures of the three natural UV protectants**;** quercetin, retinol and p-coumaric acid mentioned in the article.

Explain why these molecules are all able to absorb UV radiation.

2. The LC_{50} of a chemical is a measure of the toxicity of that chemical. It is the lethal dose in which 50% of the population is killed in a given time period.

   A recent study reported the LC_{50} for planulae, the larval form of the coral *Stylophora pistillata,* exposed to oxybenzone in the light over an 8 h period to be 3.1 mg/L.

   1000 mg = 1 g; 1 L = 1 dm^3

   a. Calculate the molar mass of oxybenzone.

   b. Determine the LC_{50} of oxybenzone in units of mol/dm^3.

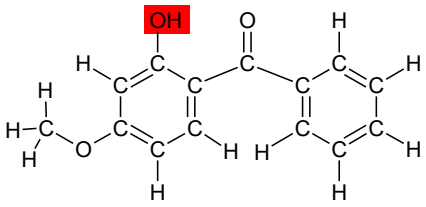
Answers

1. a. Highlight the following functional groups on the structures given in **Figure 1**;

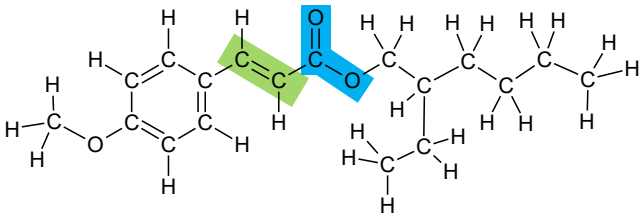
   i. alkene NOTE It might be worth introducing students to benzene rings at this point

   ii. alcohol

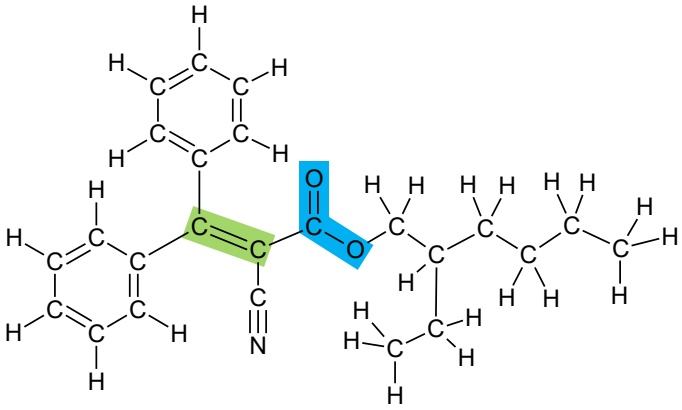
   iii. ester



oxybenzone



octinoxate



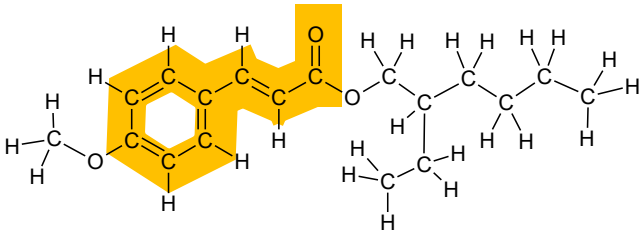
octocrylene

   b. i. They both contain a 6 membered ring with an OCH_3 group attached on the same carbon.

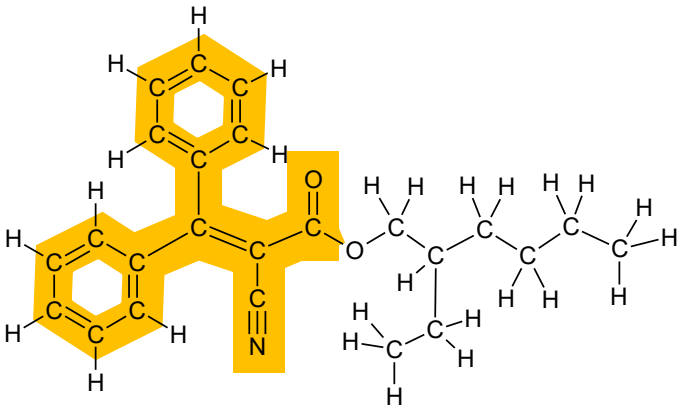
   ii. They both contain the same alkyl group attached to the ester group i.e. the part of the molecule on the right is the same.

   They also both contain a six membered ring connected to an alkene connected to the C=O of the ester group.

   c. **octinoxate**



octocrylene



2. a. Molecular formula of oxybenzone $C_{14}H_{12}O_3$

   Molar mass of oxybenzone (14 × 12.0) + (12 × 1.0) + (3 × 16.0) = <u>228.0 g/mol</u>

   b. 3.1 mg/L = 0.0031 g/L = 0.0031 g/dm^3 = $\left(\frac{0.0031\ g}{228.0\ g/mol}\right)$ / dm^3 = <u>1.36 × 10^{-5} mol/dm^3</u>