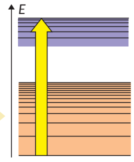
Solvatochromism

Sek. II

The solutions of the *same* substance in *different* solvents differ in colour



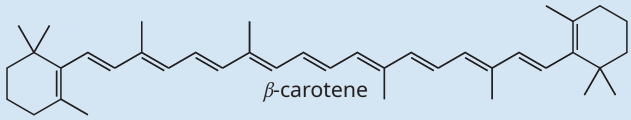
required previous knowledge	intermolecular forces (IMFs)	chemical equilibrium	electron energy diagram	light spectrum and light absorption	chemical polarity	molecular structure and colour

Basic experiment and analysis assignments for all groups

Group 1: Structure and colour

S1 Mark the chromophore as well as auxochrome(s) and anti-auxochrome(s) in the structural formulae of spiropyrane and merocyanine. Give reasons for the fact that the dissolved spiropyrane is colourless.

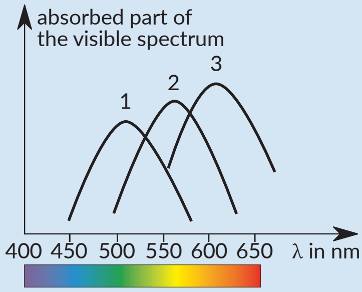
S2

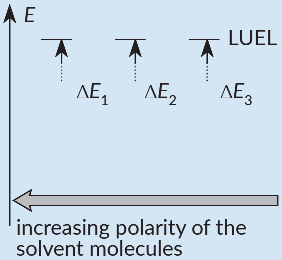


The orange *β*-carotene absorbs blue light (λ_{max} = 444 nm) and the blue merocyanine absorbs yellow light (λ_{max} = 600 nm). Compare the length of the chromophore in the two molecules and deduce the influence of the auxochrome(s) on the light absorption.

S3 Draw a resonance structure of the given merocyanine zwitterion and assess which of the two resonance structures is more likely to be found in a polar solvent.

Group 2: Energy level diagram





E1 Assign the three absorption maxima of merocyanine to the three used solvents. Give reasons for your choice.

E2 With the help of E1, draw the **h**ighest **o**ccupied **e**nergy **l**evel HOEL for the merocyanine-molecule in each of the three solutions into the right diagram.

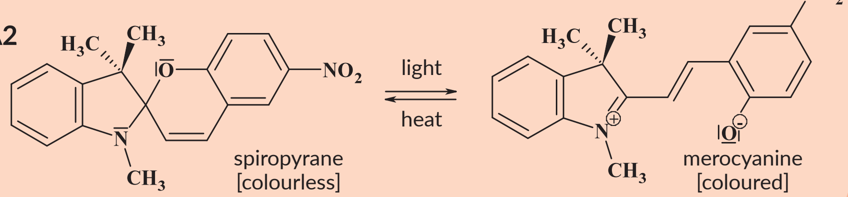
E3 Carry out some research into the concepts of *bathochromic* and *hypsochromic shift* as well as the concepts of *positive* and *negative solvatochromism*. By means of your findings, explain your observations.

Experiment

Dissolve 5 mg of spiropyrane in three different test tubes in 5 mL of xylene, acetone, and ethanol, respectively. Irradiate each of the three solutions with the violet LED torch for one minute. Note down all your observations and store the samples in a dark place.

A1 Write down the structural formulae of the three solvent molecules and compare their chemical polarities. Justify your findings with the appropriate chemical terminology.

A2



Identify the differences between the two molecules spiropyrane and merocyanine. Use the following attributes and explain your decisions: *molecular formula*, *chemical polarity*, *length of chromophore*, *molecule's planarity*.

A3 Develop a hypothesis for the explanation of the different colours of the three solutions.

Group 3: Chemical equilibrium

C1 Formulate a chemical equilibrium constant for the spiropyrane-merocyanine-equilibrium.

C2 In the dark, chemical equilibria have been reached in the three different solutions. Estimate the ratio of the merocyanine molecules, which are responsible for the colour of the solution, in xylene and ethanol. Afterwards, formulate a rough mathematical relation between the two equilibrium constants ("bigger than"/"smaller than").

C3 Measure the time the spiropyrane-merocyanine-equilibrium in xylene needs to settle after switching off the violet LED torch. How much time will the same solution need at 0 °C and 50 °C? Propose a hypothesis and test it out by way of experiments.

Group 4: Nano-environment

N1 Draw structural formulae showing the intermolecular interacions within the three different solutions. Doing so, include and name the intermolecular forces between a merocyanine-molecule and the respective solvent molecules.

N2 Look again at the solutions which have been stored in a dark place after the irradiation in the basic experiment. On the basis of the colours decide whether there is only spiropyrane within the solutions – or if there is some merocyanine, too.

N3 Formulate a '*The ..., the ...*'-statement in order to point out the correlation between the polarity of the nano-environment, i.e. the solvent molecules, and the stabilization of the merocyanine-zwitterion.