DETERMINATION OF DIPOLE MOMENT OF ACETONE

OUTLINE

In this experiment values of the dielectric constant and the refractive index of several acetone-cyclohexane solutions will be measured. On their basis, the value of the acetone dipole moment will be calculated.

INTRODUCTION

If in a molecule the centers of positive and negative electric charges of atoms or functional groups do not overlap, this molecule has a **permanent dipole moment** $\boldsymbol{\mu}$. Moreover, within each molecule under the influence of the external electric field, an **induced dipole moment** will be found, described by the equation:

$$\mu_{ind} = \alpha_e E + \alpha_a E \tag{1}$$

where:
α_e - denotes electronic polarizability
α_a - denotes atomic polarizability
E - the intensity of the electric field

Thus, generally, a molecule placed under the influence of an external electric field has a dipole moment μ' equal to:

$$\mu' = \mu + \mu_e + \mu_a = \mu + \alpha_e E + \alpha_a E \tag{2}$$

The Clausius-Mosotti equation connects the polarization of a dielectric material ***P*** with the value of its dielectric constant $\boldsymbol{\varepsilon}$ and with the permanent dipole moment $\boldsymbol{\mu}$ based on the equation:

$$P = \frac{(\varepsilon - 1)}{(\varepsilon + 2)} \cdot \frac{M}{d} = \frac{N}{3\varepsilon_o}\left(\alpha_{ind} + \frac{\mu^2}{3kT}\right) \tag{3}$$

where:
M - molecular mass of the dielectric
d - density of the dielectric
N - Avogadro constant
k - Boltzmann constant
ε_o - dielectric permittivity of vacuum
ε - dielectric permittivity

The expression defines the so-called **orientation polarization** (a component of the permanent dipole moment aligned towards the field). Orientation polarization is found only in static fields or at relatively low frequencies. At high frequencies of the external electric field, we deal only with **induced polarization**. The electromagnetic wave in the visible region has an electric component with a sufficiently high frequency to prevent orientation polarization. The refractive index approximately meets the ***Lorentz-Lorenz relation***:

$$n^2 = \varepsilon \tag{4}$$

Based on the presented considerations we define the function termed refraction, ***R***, with the following equation:

$$R = \frac{(n^2 - 1)}{(n^2 + 2)} \cdot \frac{M}{d} = \frac{N}{3\varepsilon_o} \alpha_{ind} \tag{5}$$

Polarization is equal to refraction plus the factor connected with the presence of a constant dipole moment:

$$P = R + \frac{N\mu^2}{9kT\varepsilon_o} \tag{6}$$

from which we derive the equation, which based on known values of *P* and *R* produces the value of μ :

$$\mu = \sqrt{\frac{9kT\varepsilon_o}{N} T(P - R)} \tag{7}$$

The dependencies given above are correct for an ideal gas, i.e. for a system, in which apart from thermal there are no other interactions. To eliminate these interactions in a real system, measurements need to be taken using solutions of the tested compound (e.g. acetone) in diluted solutions in a neutral solvent (e.g. cyclohexane).

Polarization of a solution, P_{12}, meets the dependence:

$$P_{12} = x_1 P_1 + x_2 P_2 = \frac{M_{12}}{d_{12}} \cdot \frac{(\varepsilon_{12} - 1)}{(\varepsilon_{12} + 2)} \tag{8}$$

where indexes 1 and 2 refer to the solution, index 1 to the solvent, while index 2 - to the solute (the analyte; symbol x denotes the mole fraction.

The molecular mass of a solution, M_{12}, is given by the expression:

$$M_{12} = x_1 M_1 + x_2 M_2 \tag{9}$$

Analogously, this dependence is correct for refraction

$$R_{12} = x_1 R_1 + x_2 R_2 = \frac{M_{12}}{d_{12}} \cdot \frac{(n_{12}^2 - 1)}{(n_{12}^2 + 2)} \tag{10}$$

Knowing measured values of R_1, P_1, R_{12} and P_{12} we may calculate the values of R_2 and P_2 for solutions with varying concentrations of the solute (x_2).
Graphical extrapolation of R_2 and P_2 values to an infinite dilution in the system $R_2(P_2) = f(x_2)$ makes it possible to determine the values of R_2 and P_2 for a system, in which interactions between molecules do not take place. Values of R_2 and P_2 determined by extrapolation make it possible to determine the value of the dipole moment of the solute. Values required in the equations may be determined based on the measurement of the capacity of:
- an air condenser (using air or solvent vapors), c_3,
- a solvent-based condenser, c_1,

- a condenser containing a solution, c_{12}
and the equation:

$$\varepsilon_{12} = \frac{c_3 - c_{12}}{c_3 - c_1} \cdot (\varepsilon_1 - 1) + 1 \tag{11}$$

Assuming that the capacity of the connectors is negligible and that the condenser not filled with a liquid (i.e. ‘empty’) has a capacity equal to the capacity of the condenser in vacuum (c_o), equation (11) is simplified to the commonly known form;

$$\varepsilon_{12} = \frac{c_{12}}{c_o} \tag{12}$$

For these calculations, we need the value of the dielectric constant of the solvent, ε_1, which for the solvent (cyclohexane) is **2.02**. The density for the solvent d_1 and solution d_{12} may be determined using a pycnometer.

PURPOSE OF EXERCISE

- Determination of the dipole moment of acetone from relative permittivity and refractive index.

APPARATUS

- Radelkis OH-301dielectrometer.
- a capacitor.
- an Abbe refractometer.
- a dryer.

GLASSWARE

- a pycnometer.
- a 1 cm^3 pipette.
- a 150 cm^3 beaker.
- a porcelain tray.

CHEMICALS

- Cyclohexane.
- 6 solutions of acetone in cyclohexane with increasing acetone content.

EXPERIMENT PROCEDURES

1. Measurement of condenser capacity:

The test condenser consists of two concentrically arranged metal cylinders, one of which constitutes a casing, and the other, a smaller one is placed inside it. The whole device is equipped with a valve so that the solution found inside may be evacuated.
Dry the walls with cool air from the dryer. Next measure the capacity of the empty condenser, c_3, using a dielectrometer. Following the measurement check if the cock valve located in the bottom part of the condenser is closed. To measure the capacity of a condenser filled with cyclohexane or a respective

solution it needs to be poured into the condenser so that the liquid covers the internal cylinder being one of the condenser cases. Capacities c_1 and c_{12} need to be measured in the following order: cyclohexane, solutions with the acetone concentration series from the lowest to the highest. After measurements are completed the condenser (its walls) needs to be washed with a small amount of cyclohexane, which needs to be poured out to a special laboratory liquid waste container located near the laboratory bench. Liquids used in measurements (cyclohexane and serial dilutions) need to be poured into a beaker (after each measurement) by opening the bottom cock and next **poured into the bottles, from which they were collected.**

2. Measurement of the refractive index:

This measurement needs to be performed in the same order as the previous one, i.e. cyclohexane followed by solutions with an increasing acetone concentration.

3. Measurement of density:

The pycnometer needs to be filled and closed over a porcelain cuvette, in which slight amounts of excess liquid will be collected. After filling the pycnometer has to be wiped with blotting paper. After the measurement is completed, the liquid from the pycnometer needs to be poured into the bottle, from which it was collected.

CAUTION!!!
DO NOT RINSE the condenser, the pycnometer, the pipettes, and used laboratory glassware with water.

PREPARATION OF RESULTS

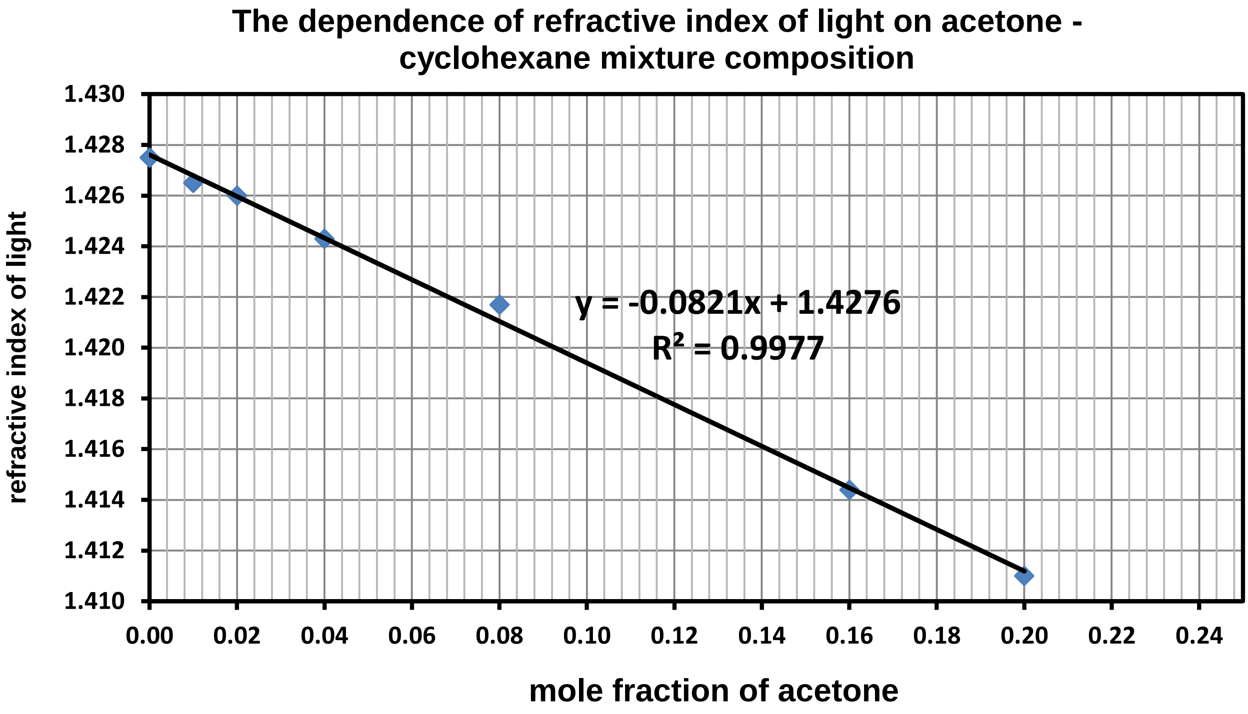
1. Read acetone content (the mole fraction) from the analytical curve based on measurements of the refractive index.

2. Present in tabular form the measurement results for the capacity of the empty condenser and the condenser filled with cyclohexane and serial dilutions, the refractive index of cyclohexane and acetone solutions, as well as the weight of the empty pycnometer, the pycnometer containing cyclohexane and acetone solutions.

3. Based on measured values calculate the values of polarization (P_{12}) and refraction (R_{12}) for individual solutions. Knowing (R_1), (P_1), (R_{12}), and (P_{12}) values calculate values of (R_2) and (P_2) for solutions with varying concentrations of the solute (x_2).

4. Plot the graph for the dependence of polarization (P_2) and refraction (R_2) of the solutions on acetone concentration. Determine polarization (P) and refraction (R) of acetone by extrapolation.

5. Calculate the value of the dipole moment of acetone using equation (7).


The dependence of refractive index of light on acetone - cyclohexane mixture composition
refractive index of light
1.430
1.428
1.426
1.424
1.422
1.420
1.418
1.416
1.414
1.412
1.410
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20
0.22
0.24
y = -0.0821x + 1.4276
R² = 0.9977
mole fraction of acetone

Template of the table and draft of the study

……………………………... *Faculty* ……………………………….. *Field of study* *Full-time/ part-time studies*	……………………………………………… *Name and surname*	…………………………………... *Date:*
Group no.: ………………… *Team no.:* …………………	……...…………… *Exercise no.:*	…………………………………….. *Instructor:*

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Nr grupy: …………………... *Nr zespołu:* …………………..	……...…………… *Nr ćwiczenia:*	…………………………………….. *Nazwisko Prowadzącego:*

1. Temat ćwiczenia
2. Cel ćwiczenia:
3. Wstęp teoretyczny:
4. Pomiary:
5. Obliczenia:
6. Wykresy:
7. Wnioski

1. Exercise title:
2. The aim of the exercise:
3. Theoretical introduction:
4. Results:
5. Calculations:
6. Graphs:
7. Conclusions: