



Traditio et Innovatio

## **Book of Abstracts**

# **THERMAN 2020**

9<sup>th</sup> Rostocker International Conference: "Technical Thermodynamics: **Thermophysical Properties and Energy Systems**"

Institute of Technical Thermodynamics

University of Rostock, **Rostock, Germany** 

15 October 2020

INSTITUTE OF TECHNICAL THERMODYNAMICS

9th Rostocker International Conference: "Thermophysical Properties for Technical Thermodynamics", 15 October 2020, Rostock, GERMANY



# THERMAM 2020

## 9th ROSTOCKER INTERNATIONAL CONFERENCE: "TECHNICAL THERMODYNAMICS: THERMOPHYSICAL PROPERTIES AND ENERGY SYSTEMS"

15 October 2020

University of Rostock Albert Einstein Str. 2

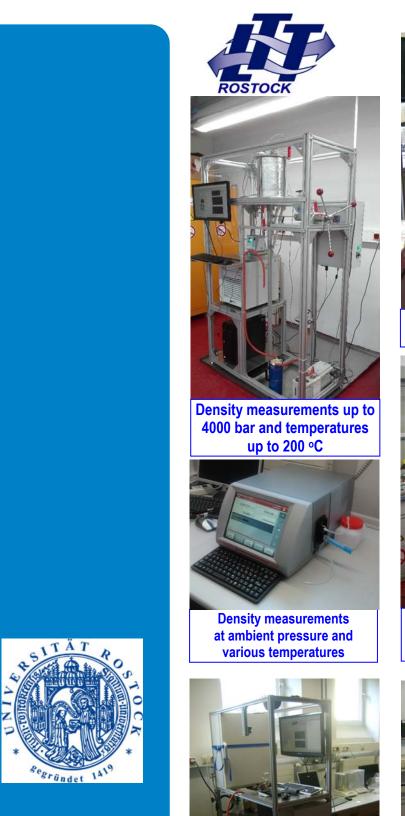
**Rostock, GERMANY** 



## **IN COOPERATION:**

Institute of Hydraulic and Heat Techniques, Azerbaijan Technical University, Baku, **AZERBAIJAN** Institute of Petrochemical Processes named after Yu.G. Mamedaliyev of ANAS, Baku, **AZERBAIJAN** Institute of Mechanical Engineering, Dokuz Eylul University, Izmir, **TURKEY** Institute of Food Engineering, Ege University, Izmir, **TURKEY** 

2020





Vapor pressure measurements at high temperatures



**Density measurements** up to 1400 bar and temperatures up to 200 °C



Vapor pressure measurements at small temperatures



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Gas solubility measurements in liquids at high pressures and wide range of temperatures

## **BOOK OF ABSTRACTS**

## 9th ROSTOCKER INTERNATIONAL CONFERENCE: "TECHNICAL THERMODYNAMICS: THERMOPHYSICAL PROPERTIES AND ENERGY SYSTEMS"

## **THERMAM 2020**

15<sup>th</sup> October 2020

University of Rostock Albert Einstein Str. 2, D-18059 Rostock, GERMANY

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## Preface

### 9th ROSTOCKER INTERNATIONAL CONFERENCE: "TECHNICAL THERMODYNAMICS: THERMOPHYSICAL PROPERTIES AND ENERGY SYSTEMS"

Thermodynamics is a very fascinating scientific field, which has to do with many different phenomena in nature and technique. As an interesting example, we can regard climate change, which at the moment is on the agenda of many political decision makers and scientists. Climate change is partly caused by the emission of the carbon dioxide molecule to the atmosphere from farming, from technical combustion in energy technique and transport and from many other human related processes. The heat transfer processes within the atmosphere clearly involve thermodynamics. On the other hand, measures to reduce human impact on the environment, like CCS, carbon capture and storage, from combustion also involve thermodynamics processes. To solve and handle thermodynamic problems one needs "Thermophysical and Mechanical Properties of Advanced Materials". One example is the possible capture of carbon dioxide from the atmosphere or exhaust gases in ionic liquids. To make this technically feasible, data on the thermophysical property of carbon dioxide solubility in the advanced material of an ionic liquid are needed.

With this conference we want to bring together international scientists and engineers, who work in the very broad field of "Thermophysical and Mechanical Properties of Advanced Materials". This is a very interesting and modern research field. It covers experimental and theoretical new results for thermophysical properties, new measurement techniques and their applications, molecular modeling with new theoretical insights, applications which show the improvement done with the described research for thermophysical properties and mechanical properties for materials like nanofluids, nanocomposites, alternative solvents, metals, alloys, ceramics, composites, etc. These subjects cover fundamental and applied research and engineering aspects.

We want to foster lively discussions and future international collaborations on this important and stimulating field with this conference.

Even though the COVID-19 pandemia leads to this years THERMAM conference been held only online, this symposium will open many opportunities for scientific exchange. This new format will enable discussions in a new way, which might also show possibilities for the future.

We wish you all an interesting, pleasant and stimulating conference and hope to meet you again next year.

#### THE ORGANIZING COMMITTEE

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## **Keynote Presentation**

#### SUBSTANCE PROPERTIES FOR ENERGY TECHNOLOGIES

#### Karsten MÜLLER

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**Prof. Dr.-Ing. habil. Karsten MÜLLER** is professor and chair of the institute of Technical Thermodynamics at the University of Rostock in Germany. He studied chemical engineering at the Technische Universtät München (Germany) and the University of Cape Town (South Africa). After graduating in 2009 he moved to the Friedrich-Alexander-Universität Erlangen-Nürnberg, where he received his PhD in 2013 for a thesis on CO<sub>2</sub> utilization. In 2018 he received is habilitation at the same university for his works on energy storage technologies. Before accepting the position as professor in Rostock, he conducted further research at the Pacific Northwest National Laboratory (USA) and the Forschungszentrum Jülich (Germany).



Thermochemical and thermophysical properties of working substances can have a tremendous effect on the performance of energy technologies. Particularly favored by the emerging of renewable energies, the importance of energy storage has drawn much attention in recent years. Basically all energy storage technologies operate on chemical substances. Selecting these substances properly with respect to their properties can yield significant improvements.

However, the effect of different properties on the overall performance can vary. The potential of different parameters for improving systems can be identified using suited techniques [1]. It can be demonstrated that there are applications for which thermodynamic properties can have a larger impact on improving system performance than improving the apparatuses involved. Yet, the impact of different properties can be very different and in some cases there are still namable potentials related to apparatuses. Hence, proper system analysis is mandatory to identify the thermodynamic properties with the highest potentials for improvement.

In this presentation, an overview will be given on these analyses as well as on developments in measurement of thermophysical properties at the *Institute of Technical Thermodynamics* of the *University of Rostock*.

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## **Oral Presentations**

#### PHYSICAL AND CHEMICAL PROPERTIES AND COMPOSITION OF EXHAUST GASES OF DIESEL-ETHANOL-EMULSIFIER MIXTURES

#### Vaqif ABBASOV<sup>1</sup>, Tarana MAMMADOVA<sup>1</sup>, Sevinj MAMMADKHANOVA<sup>2</sup>, <u>Adil ABBASOV<sup>2</sup></u>, Tarana LATIFOVA<sup>1</sup>

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The limited oil resources and the tightening of the environmental measures of both the fuels and their combustion products makes it necessary to use alternative types of raw materials for the production of motor fuels, such as bioethanol and other alcohols. This article presents the results of obtaining the diesel fuel with a content of up to 5% watered and dehydrated ethanol. Experiments on the production of diesel-ethanol compositions were carried out at the temperature range of 0–25 °C with mixing of mixtures using a rotary mixer and an ultrasonic sonotrode with an oscillation frequency of 20 kHz. It was revealed that the stability of diesel-alcohol compositions on using dehydrated ethanol in the composition of diesel fuel to 3% mass. at room temperature is 30 days. The increase of the ethanol content in the diesel fuel composition reduces the stability period of obtained mixture to 25 and 18 days, respectively. For low temperatures, the reduction at the period of stability of the compounds is up to 10 days for 1-2%, 8-5 days for 3-5% compounds, respectively.

On using watered ethanol, even when it is contained in diesel fuel 1% during mixing with an agitator with a turnover rate of 600 rpm, an unstable emulsion forms, which stratifies after a few minutes. The increase of ethanol content in composition of diesel fuel leads to the formation of an even less stable emulsion. However, on mixing the obtained compounds using an ultrasonic sonotrode, slightly coalescing mixtures are formed, the stability of which is no more than 10 days at room temperature and 5 days at low temperature.

Using the method of dynamic light scattering, the dynamics of changes in the size of droplets of watered ethanol in diesel fuel composition with time was investigated and it was established that on the day of preparation of compositions the size of ethanol drops in diesel fuel composition for 3% compound at room temperature is 150-160 nm. On the 5th day after preparation of the compound, the particle size of ethanol increases to 800-900 nm, after which there is a rapid separation of the mixture into diesel and ethanol layers.

To preserve the emulsion of diesel fuel using watered ethanol, an emulsifier obtained on basis of petroleum acids and propylene oxide have been used. Revealed that the addition of it to the composition of the 3% composition of ethanol with diesel fuel ensures the production of homogeneous diesel fuel with retention of all its normalized parameters. The particle size of ethanol in the diesel fuel composition on the day of preparation is 2-7 nm, on the expiry of 20 days the ethanol droplet size increases to 80-90 nm, which ensures the long-term stability of the obtained compound.

It was revealed that, despite the water content of ethanol, the use of this emulsifier ensures the production of homogeneous diesel fuel while retaining all its normalized measures. Reducing the content of carbon monoxide, sulfur oxides and nitrogen in the composition of exhaust gases is 28%, 24% and 16%, respectively.

#### EXPERIMENTAL STUDY OF THE *PVTx* PROPERTIES OF BINARY WATER + *n*-HEXANE AND TERNARY WATER +1-PROPANOL + *n*-HEXANE MIXTURES IN THE CRITICAL AND SUPERCRITICAL REGIONS

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The liquid-liquid-gas (LLV) and liquid-gas (LV) phase transition ( $p_s, T_s, \rho_s, x$ ) and ( $p, T, \rho, x$ ) properties of binary (water+n-hexane) and ternary (water+1-propanol+n-hexane) mixtures with fixed concentration were measured using high-temperature and high-pressure constant-volume piezometer technique. Measurements were focused in the immediate vicinity of the critical and supercritical regions in order to closely observe the features of the mixture critical behavior. Measurements were made for equimolar binary mixture (0.5 mole fraction of n-hexane) water+nhexane over a temperature range from (373.15 to 673.15) K and pressures between (0.25 and 56) MPa. The measurements were performed for 15 liquid and vapor isochores between (55 and 554) kg·m<sup>-3</sup>. For the ternary mixture the measurements were made along 29 liquid and vapor isochores between (25.03 and 646.59) kg·m<sup>-3</sup> and over the temperature range from (373.15 to 673.15) K at pressures up to 60 MPa. For each isochore most measurements were focused in the immediate vicinity of the LLV and LV phase transition temperature (in the single-, two-, and three-phase regions) where the break of the P-T isochore's slopes are observing. Temperatures and pressures  $(T_s, \rho_s)$  at the LLV and LV phase transition points for each fixed density (isochore,  $\rho$ ) were measured using the isochoric *p*-*T* break point technique in the immediate vicinity of the critical point of the mixtures. The upper critical end point property data ( $T_{UCEP}$  = 469.15 K,  $p_{UCEP}$  = 5.229 MPa, and  $p_{UCEP}$  = 263.95 kg·m<sup>-3</sup>) for the binary and ( $T_c$  = 510.85 K,  $p_c$  = 6.09 MPa, and  $\rho_c$  = 255.22 kg·m<sup>-3</sup>) for the ternary mixture were extracted from the detailed  $(p,T,\rho,x)$  and  $(p_s,T_s,\rho_s)$  measurements in the immediate vicinity of the critical point. The combined expanded uncertainty of the density,  $\rho$ , pressure, p, temperature, T, and concentration, x, measurements at the 95 % confidence level with a coverage factor of k = 2 is estimated to be 0.2 % (density in the liquid phase), 0.3 % (density in the gas phase); 0.5 % (density in the critical and supercritical regions); 0.05 % (pressure), 15 mK (temperature), and 0.01 mole % (concentration). The excess molar volumes ( $V_m^E$ ) of the binary and ternary mixture were calculated using the measured molar volumes V<sub>m</sub> of the mixtures and well-known reference molar volumes of the pure components for various experimental temperatures and pressures in the supercritical region. Also, the measured  $(p, T, \rho, x)$  data at low densities (vapor phase) were used to calculate the theoretically meaning properties such as second and third virial coefficients of the mixture at high temperatures.

#### ACKNOWLEDGEMENTS

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#### THERMAL CHARACTERISTICS IMIDAZOLINE-MODIFIED ALKYL PHENOLFORMALDEHYDE OLIGOMERS

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The thermal stability of alkyl phenolformaldehyde oligomers (APhFO) modified with imidazolines based on acids isolated from soybean oil and polyamines in various molar ratios (with diethyleneamine 1:1, triethyleneamine 1:1, polyethylenepolyamines 1:1 - 2:1) was studied by thermogravimetric analysis. The studies were carried out on a (TG / DTG / TG / DTA) YUPITER STA 449 F3 thermal analyzer of the German company NETZSCH in an inert nitrogen atmosphere in the temperature range 25-650 °C with an increase in temperature in increments of 10K/min. Their thermal features were determined depending on the composition. The results obtained were compared with the corresponding indicators of unmodified APhFO. It was found that APhFO modified with imidazolines based on soybean oil with polyamines, in contrast to unmodified compounds, undergoes destruction in stages. So the destruction of unmodified APhFO was observed in one stage, mainly in the range of 337.9-403.7 °C, and the destruction of modified APhFO was observed in two stages. The temperature interval recorded in the first stage, combining to the instance indicated above corresponds to the allocation of additional mass, the highest value being in the range of 57.6-272.5 °C. This corresponds to a very small mass loss. The highest value of the onset of sensitive destruction was observed at 272.5 °C. The second stage of destruction ends in the range 547.7-646.4 °C. The maximum temperature at which the destruction occurs varies between 506.7-562.3 °C. For a sample of AFFO modified with imidazoline based on an acid isolated from soybean oil with PEPA in a 2:1 molar ratio, this stage is absent. The temperature interval at which the 2nd stage occurs is slightly higher than the destruction interval of unmodified APhFO. The maximum temperature of destruction also gets a definitely high value. These comparisons show their highest thermal resistance. Presumably, this stage is associated with the breaking of the alkyl phenolphormaldehyde chain and is observed in all samples with small displacements. Apparently, in the temperature range indicated in the second stage, the possibility of breaking in the polyamine chain is not excluded. Despite the fact that there is no sharp regularity in the change in the values of the heat areas, in the temperature interval of the corresponding second stage, an increase is mainly observed. Given the foregoing, the following hypotheses can be put forward:

- Thermal destruction of all the studied samples begins at 300 °C and reaches significant results at 500-600 °C. At temperatures above 600 °C it stabilizes,
- The thermal stability of APhFO -modified imidazolines in comparison with non-modified APhFO is higher,
- Loss of mass is accompanied by endo-effects that prove destruction and this occurs mainly in the range of 200-300 °C,
- Presumably, the second stage of destruction is accompanied by the cleavage of the alkyl phenol formaldehyde and polyamine chains,
- The complex structure of the modified oligomers determines their multi-stage destruction.

#### MEASUREMENT OF HEROIN AND ITS METABOLITES IN SALIVA USING SURFACE ENHANCED RAMAN SPECTROSCOPY

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**Background:** Heroin can be detected and quantified by certain analytical methods; however, forensic professionals and criminal laboratories study for cheaper and faster detection tools. Surface-enhanced Raman spectroscopy rise as a possible alternative tool with its widening application spectra. There are few studies regarding Raman and SERS spectra of heroin and its metabolites, which are unfortunately controversial. In this study we compared five different surfaces in order to find out more efficient Raman-active substrate for opiate detection and rapid quantification of heroin and its metabolites in saliva.

**Methods:** Morphine standard material was used to identify proper surface for SERS analysis of opiates. Heroin and its metabolites (morphine, morphine-3-ß-glucuronide and 6-monoacetyl morphine) were calibrated between 50 ppb and 500 ppm and quantified on AuNRs with signal enhancement of silver colloids in saliva. Raman microscope with a 785-nm laser source was used.

**Results and Conclusion:** Obtained results showed that heroin and its metabolites can be detected and quantified in saliva samples using a SERS-based system. Additionally, the present study revealed that synergetic effect of a specific gold nano-surface with ability controlling liquid motion and silver nanoparticles increase band numbers and intensities. Therefore, we suggest a fast, accurate and cost-effective method to detect and quantify heroin in biological fluids.

**KEYWORDS:** Heroin and morphine identification, Heroin and morphine quantification, surface-enhanced Raman spectroscopy (SERS), Raman-active surface, gold nanorod arrays, silver nanoparticles.

#### T-X AND P-T-X PHASE DIAGRAM OF THE Cu-Pb-S SYSTEM AT HIGH TEMPERATURES

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The phase diagram of the Cu-Pb-S system is of interest for pyrometallurgy and semiconductor materials science. In pyrometallurgy, data on phase equilibria at various temperatures are needed to determine the conditions for obtaining pure copper from sulfide concentrates suitable for use in electrical engineering. If in pyrometallurgy the task is to clean copper concentrates from harmful impurities of lead, then in the semiconductor technique the problem of producing lead and copper sulfides by crystallization from liquid alloys and the gas phase Cu-Pb-S is solved. In this work based on the thermodynamic calculation, the boundaries of the immiscibility of liquid alloys of the Cu-S, Pb-S, and Cu-Pb-S systems were first determined and analytically described using literature data and the experimental results of this work. To determine the boundaries of the liquid immiscibility, the thermodynamic condition of the internal phase stability ( $\partial^2 G/\partial x^2$ )<sub>P,T</sub>>0 was used. Critical temperatures and pressures for immiscibility regions of liquid alloys are characterized by high values: T<sup>kr</sup>=1520÷1920K; P<sup>kr</sup> =170 ÷ 510 atm. The crystallization surfaces of lead sulfide with electronic conductivity (p-type PbS) and with hole conductivity (n-type PbS) are calculated and analytically described, as well as the corresponding values of sulfur vapor pressure over the crystallization surface of lead sulfide. All analytical dependencies for 3D modeling were obtained and visualized using the OriginLab computer program. In particular for 3D modeling of the P-T-x phase diagram of the ternary Cu – Pb – S system, the following dependences were obtained (all equations are presented in computer variation):

$$\lg p_{S_2}$$
 (atm,Cu-Pb-S, p-type PbS)= 64-320\*y+487\*y^2-232\*y^3-3.84\*x (1)

$$\lg p_{S_2}$$
 (atm, Cu-Pb-S, n-type PbS) = 1836-6844\*y+8499\*y^2-3524\*y^3-5.77\*x (2)

In eq. (1,2): y=1000/T)=0.712-0.85;  $x=y_{Cu}=0-0.26$  and y=1000/T)=0.714-0.83;  $x=y_{Cu}=0-0.26$  Equations (1,2) are visualized in figure:

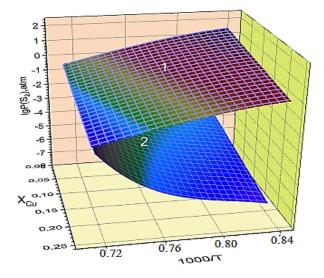


Figure. 3D model of the PTX diagram for isolines of the partial pressure of saturated vapor  $S_2$  over the surface of the PbS liquidus in the ternary system Cu-Pb-S, visualized by equations 1.2. 1-region PbS-S (p-type conductivity), 2- region PbS-Pb (n-type conductivity).

#### PREPARATION OF NOVEL CHEMICAL MATERIAL FOR SAND CONSOLIDATION

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Sand particle production is a problem that can be encountered in many reservoirs worldwide. Today, a wide variety of sand control methods are available with various levels of complexity and applicability. The main object of this paper is to present a suitable resin to be used as a consolidating agent in the oil fields. Considering economically affordability and required desirable characteristics of resins for the consolidation process is a prepared epoxy resin based on Bisphenol-A.

The development of sand control techniques is progressing in the oil industry. Several methods comprising mechanical and chemical methods of sand consolidation have been developed by different researchers. This paper comprehensively commentary the mechanism of sand formation and control, various investigations and techniques used in the chemical sand consolidation process. In this work epichlorohydrin, Bisphenol A, amines, poly(ethylene glycol) diglycidyl ether, organosilane compounds and nanoparticles are using for sand consolidating material. The ratio of the compounds used is estimated based on the modelling, taking into account the required viscosity, temperature and other characteristics.

The epoxy resins have at least two reactive epoxy groups in their molecule and n is an integer having a value of 1 or a greater number. Also used curing agents, known as hardeners for the thermosetting resin. The hardeners have the property of catalyzing the hardening reaction of the thermosetting resin at low temperatures. The preferred epoxy resins may be cured or hardened with a direct linkage between the epoxy groups by the use of amines and organosilane compounds. Organosilane compound contains an amino group. Moreover, in this work, we used polyfunctional organosilane compound. Polyfunctional organosilane compound utilized for increasing adhesion of the epoxy resin. The purpose of using nanostructures is to increase the adhesion of chemicals. Toluene, xylene or isopropyl alcohol was used as a solvent in the preparation of epoxy resin solutions and hardening agent solution. It is intended to use modelling to determine the density, viscosity and other parameters which required for in-situ application of the prepared solutions.

This laboratory research was carried out to preparation of new material for chemical sand consolidation and investigate the capacity of new material to consolidate the loose sand under the reservoir condition. The modelling consequences give the expected results in laboratory tests, suggesting that the material will be successfully applied in-situ.

#### 3D HELMHOLTZ COIL SYSTEM DESIGN FOR MEASURING THE THERMAL CONDUCTIVITY OF MAGNETIC NANOFLUIDS

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Magnetic nanofluids are colloids that contain nanosized particles with magnetic properties dispersed into a base fluid to improve the thermophysical properties of the base fluid. These fluids have many possible application areas such as biomedical and heat transfer because their thermophysical properties can be altered under applied magnetic field. One of the thermophysical properties that can be altered using an external magnetic field is thermal conductivity of these fluids. The studies on the measurement of the thermal conductivity of the magnetic nanofluids put emphasis on the direction and the uniformity of the magnetic field applied to the fluid as the results show that thermal conductivity results change when the external magnetic field is applied parallel or perpendicular to the temperature gradient of the thermal conductivity measurement probe. Permanent magnets and electromagnets are commonly employed in these studies and the direction changes are made mechanically as the field is applied only in two directions. The proposed design enables to measure the thermal conductivity of the magnetic field generator. By using the rotating magnetic field, the external magnetic field can be applied in any desired direction. These systems allow us to investigate the effect of the magnetic field more thoroughly and effectively.

Keywords: 3D Helmholtz coil, magnetic field, magnetic nanofluids, thermal conductivity.

#### ACKNOWLEDGMENTS

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#### USING THE JULIA PROGRAMMING LANGUAGE TO CALCULATE THE EQUILIBRIUM COMPOSITION OF A MULTICOMPONENT GAS PHASE SYSTEM

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The problem of calculation the equilibrium composition of chemically reacting thermodynamic systems has long attracted the attention of many researchers, since it has a significant applied value. The first computer-oriented algorithms for solving this problem were proposed back in the 50s of the last century. But the problem is still relevant. We present here a modified algorithm for calculating the equilibrium in a multi-component homogeneous thermodynamic system, developed by Professor of Bauman Moscow State Technical University B.G. Trusov, and the corresponding function MicPV in the programming language Julia (julialang.org). We chose Julia for the implementation of the algorithm, since it is a highly efficient free programming language focused on solving scientific and technical problems.

We consider a thermodynamic system formed by a mixture of ideal gases. The state of a thermodynamic system, characterized by the invariance of parameters in time and the absence of flows under constant external conditions, is usually called equilibrium. We can assume that equilibrium is some final state to which the isolated from external influences thermodynamic system tends. The isolation condition in this case means that the rate of relaxation processes inside the system is greater than the rate of change of parameters at its boundaries. In turn, in the equilibrium state, the entropy of the isolated system is maximal. Thus, the solution of the problem of calculating the equilibrium composition assumes the need to determine the coordinates of the conditional maximum of entropy

$$S(U, V, \vec{n}) \to max,$$
 (1)

subject to the constraints of constancy of internal energy and volume, mass balance, and nonnegativity of the number of moles of substances

$$U = const, V = const, \sum_{t=1}^{k} a_{pt} n_t = b_{pt} j = 1, 2, \dots, m, n_t \ge 0, t = 1, 2, \dots, k,$$

k – the number of substances in the system, m – the number of chemical elements in the system,  $a_{ji}$  - the number of atoms of element j in the molecule of substance i,  $h_i$  - the amount of element j in the system.

One can find the text of the function, examples of the data and the use of the function for calculation of equilibrium in [1]. The function was tested using the Julia 1.3. The text of the function is small and easy to understand. It can be used both for educational purposes and for solving the applied problems.

#### REFERENCE

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#### MEASUREMENTS OF THERMAL DIFFUSIVITIES OF POLYPROPYLENE GLYCOLS AND THEIR AQUEOUS SOLUTIONS

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At present polypropylene glycols are widely used in the production of solvents, synthetic lubricating oils, plasticizers, and hydraulic liquids. Low-freezing heat-carriers on the basis of aqueous solutions of polypropylene glycols are used in systems of heating, ventilation, conditioning and some other heat-exchange equipment. Increasing the efficiency of operation of these systems requires a knowledge of thermophysical properties, in particular, heat conductivity and thermal diffusivity of heat-transfer fluids in a wide range of temperatures.

In the present work measurements were made of thermal diffusivities of propylene glycol + water, dipropylene glycol + water and tripropylene glycol + water mixtures in the temperature range from 303 K to 363 K and in a complete range of concentrations; for PPG-425 + water and PPG-725 + water mixtures (solutions with a lower critical solubility temperature) measurements were made in the temperature range from 303 K to the temperature of phase separation by the liquid-liquid mechanism.

Thermal diffusivity has been experimentally determined by the laser flash technique using LFA 457 Microflash (Netzsch). Containers of stainless steel were made for working with liquid compounds. Each of them is a cylinder with a thin bottom and a deepening at the center of the lid. Two containers were used in the experiments, which differed in the thickness of the layer of the substance under investigation: 0.33 mm and 0.4 mm. The procedure of measuring thermal diffusivity of liquids is discussed in greater detail in Ref. [1]. By our estimations the uncertainty of measurements for liquid compounds does not exceed 5 %.

The samples of the compounds studied were purchased from Sigma-Aldrich and have purities better than 97 mol.%. The solutions were made on the basis of double-distilled water.

#### ACKNOWLEDGES

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KEYWORDS: thermal diffusivity, polypropylene glycols, aqueous solutions

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#### THERMAL PROPERTIES OF STABLE NANOFLUIDS COMPOSED OF MULTI-WALLED CARBON NANOTUBES DISPERSED IN 1,2-PROPANEDIOL AND 1,3-PROPANEDIOL FOR HEAT TRANSFER APPLICATION

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The systems composed of nanoparticles dispersed in base solvent as new generation heat transfer fluids can be used in various applications such as engine coolants, solar panels, geothermal and in the electronics industry for the cooling of electronic components and systems.

The presence of nanostructures in the base fluid is capable of enhancing conventional fluid's thermal conductivity and volumetric solar-thermal conversion capability that relies on dynamic Brownian motion of nanostructures in the base fluids. The homogenously dispersed nanostructures in base liquid are required to realize the desired properties of nanofluids and to prevents clogging and abrasion issues in particular for heat-transfer channels in microelectronic devices.

The nanofluids under study are composed of in-house 16h multi-walled carbon nanotubes MWCNTs (synthesized in our laboratory via catalytic chemical vapor deposition during 16h, diameter of 60-80 nm, length of 770  $\mu$ m, BET surface of 22 m<sup>2</sup>·g<sup>-1</sup>, carbon content 98%) and 1,2-propanediol or 1,3-propanediol. The usage of nonpetroleum origin glycols provides to achive bio-based, sustainable products with highest performance and quality. The polivinylpyrrolidone was used to increase the stability of nanofluids. The dispersion were prepared by two-step procedure using non-pulsonic sonication method.

In this work thermal conductivity, density and viscosity of nanofluids are presented. The addition of MWCNTs remarkably improved thermal conductivity of nanofluids. The maximum enhancement was about 30% for nanofluids composed of 1 wt% in-house 16h MWCNTs in comparison with pure 1,2-propanediol and 1,3-propanediol.

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#### MODELLING OF SOLAR BOOSTED HEAT PUMP FOOD DRYER

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Heat pumps are heating devices utilized in various heating applications. The basic components of a heat pump is an evaporator which evaporates a refrigerant and cool the outside environment, a condenser which condenses refrigerant and heat the outside environment, a compressor which compress the refrigerant from low pressure of evaporator to high pressure of condenser, and an expansion valve which reduce the pressure from high pressure of condenser to low pressure of evaporator. Evaporator is usually transfer heat from refrigerant to an outside environment which is usually air, water or a secondary coolant such as water-ethylene glycol-water mixture. In our case outside environment is air. As evaporator, a plane metal surface is used. Evaporator pipes are attached to plate by hard brazing process. The top side of the plate is selective surface. The plate is exchange heat with air through natural convection process. Furthermore, plate is absorbed solar radiation and boosted heat transfer process so that total coefficient of performance will be much higher compare to natural convection heat transfer alone. It should be also note that sun is not a constant energy source and total radiative energy coming is changing as a function of place, time of the day and seasons. These variations should also be taken into account of the evaporator heat transfer calculations. Condenser of the system is a finned heat exchanger. Heated air in condenser is utilized in food dryer to dry fruits and vegetables. Hot air is forced through the dryer by using fans. In drying process humidity of air is an important parameter as well as the air temperature. Recirculating hot air inside of the dryer gains moisture from the drying food products. Therefore, it is controlled and above a certain level air is discharged from the frver and replace with fresh air. A recuperator unit is utilized to recover some of the heat from the discharging air. In our system modelling first phase is modelling evaporator by considering coming and absorbing and reradiating solar radiation plus natural convection effects. In refrigerant part of the evaporator, boiling heat transfer correlations will be used to define evaporating process of the refrigerant. A separate condenser, compressor, expansion valve evaporator models will be combined together with the model food dryer, including recuperator and fans and fruit drying heat and mass transfer processes. A prototype of the food dryer will be constructed and tested. As a resulting tests model will be reevaluated and improved to obtain better prediction accuracies.

#### THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES OF HUMID AIR BY USING SCHREIBER AND PITZER EOS (DRY AIR) AND IAPWS 97 (STEAM)

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In humid air thermodynamic property calculations, it is usually ideal gas EOS is used. The basic reason for this is simplicity of using ideal gas EOS. For most air condition applications it might be sufficient, but when applications with higher pressure zones are considered error level will increased. An equation of state with better accuracy of thermodynamic properties will be required for extreme cases. In this study Scheireber-Pitzer equation of state for dry air and IAPWS97 equation for water vapor will be used to establish computer programs in java language to calculate properties of humid air. Scheiber-Pitzer equation of state is a general real gas EoS form that utilized Pitzer's acentricity factor and a modified Benedict Webb-Rubin EoS. It is basically guadratic curve fitting equation to reference fluids by using Pitzer's acentricity factor as variable. A rich list of curve fitting reference fluids, including hydrocarbons and other gases, are used to obtain curve fitting coefficients. Mixing of air and water is carried out by using PR EOS mixing, but water properties such as saturation vapor pressure, saturation liquid and vapor densities are taken by utilizing IAPWS95 water and steam EOS. Basic thermodynamic and heat-mass transfer equations are used to define properties such as dew point temperature, adiabatic saturation temperature and wet bulb temperature. In order to calculate thermophysical properties such as viscosity, thermal conductivity etc. combination of cubic surface splines and Wilke, Reichenberg... methods are used. Results of developed equations are compared with Ideal gas and IAPWS-97 EOS & IAPWS G8-10 Humid air EOS and Peng-robinson EoS of humid air. A Graphical user interphase is also developed. All the program codes are listed as free access in www.turhancoban.com adress. As subprograms properties of properties of dry air and pure gas and gas mixtures can also be calculated by using set of Scheireiber-Pitzer EoS programs. All the codes are developed in java programming language.

**Keywords:** Thermodynamic properties of humid air, Scheireiber-Pitzer EoS, IAPWS95 EoS, thermodynamic properties of dry air, thermophysial properties of humid air

#### DEVELOPING FLOW CHARACTERISTICS OF NANOFLUID BASED SINGLE PHASE NATURAL CIRCULATION MINI LOOPS

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Single phase natural circulation loops are passive systems in which density gradient caused by temperature difference is the driving mechanism of heat transfer. Effects of working fluids and geometry on the stability and heat transfer performance have been widely studied and it's concluded that stable flow and highly efficient heat transfer can be achievable by miniaturization of the single-phase natural circulation loop and using nanofluids as working fluid. In this study, heat transfer performance of nanofluid based single phase natural circulation mini loop is investigated by a transient 3D numerical model. The numerical study is carried for different heater powers (10-50 W) and volumetric concentrations of Al<sub>2</sub>O<sub>3</sub>-DIW nanofluid (1-3%). Temperature difference between heater inlet and outlet, maximum temperature and effectiveness factor are used for the validation of the numerical model. It is found that performance results of transient analyses are in good agreement with experimental results in the literature and previously reported steady-state model data. In addition, the velocity and temperature distribution patterns are reported to discuss the developing flow characteristics during the initial transient phase. The overall transient behavior of the SPNCmL is also reported and compared with the available data in the literature.

#### MODIFIED HIND AND UBBELOHDE APPROACH FOR PREDICTING VISCOSITY OF BINARY AND MULTI COMPONENT LIQUID MIXTURES

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Viscosity measurements serve as a vital tool in the study of intermolecular interactions in liquid mixtures. Prediction of properties has gained a lot of significance in the past few months in light of the COVID pandemic, wherein most of the research laboratories are under lockdown and experimental work has come to a standstill. Literature survey reveals that over the years, Hind Ubbelohde equation has been considered as a very basic and an elementary predictive model. The present investigation is an attempt to modify the Hind Ubbelhode relation for prediction of viscosity. The proposed model has been tested on 150 binary, 15 ternary and 6 quaternary liquid mixtures over a wide range of temperatures. The results have been compared with other well-known predictive equations taking Average Absolute Percentage Deviation (AAPD) as the criterion for predictive capability. Grand AAPDs show that the proposed model exhibits superior predictive capability as compared to the original relation.

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#### DEGRADATION OF ALIPHATIC ALCOHOLS AT SUPERCRITICAL TEMPERATURES

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Aliphatic alcohols and their water solutions in supercritical conditions are widely used as solvents in such technological processes as supercritical water oxidation (SCWO) and supercritical fluid extraction (SCFE). Thermal stability is one of the important requirements that one must take into account in choice of solvent in supercritical conditions. The available data on the thermal stability of aliphatic alcohols and their aqueous mixtures is contradictory.

Thermal degradation of pure alcohols (methanol, ethanol, 1-propanol and 1-butanol) and water + alcohol solutions (0.2, 0.5, 0.8 mol fraction of alcohol) was studied using method of pressure increasing at a constant temperature in a closed system in a range of temperatures from 513.15 K to 643.15 K. The starting temperatures of the thermal degradation of the alcohol molecules were determined depending on their concentration in the solutions. Dependence of starting thermal degradation temperatures ( $T_H$ ) of aliphatic alcohols (methanol, ethanol, 1-propanol and 1-butanol) and their water solutions on composition (x) and number of carbon atom can be described by the next polynomial equation:

$$T_H(x) = ax^2 + bx + c$$

where x - mol fraction of alcohol; a, b, c - coefficients that depend on C. Coefficients (a, b, c) of the equation, where calculated by less square method.

#### INFLUENCE OF PARTICLE MORPHOLOGY ON THERMOPHYSICAL PROPERTIES OF CARBON-BASED IONANOFLUIDS

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Carbon-based ionanofluids (INFs) have thermophysical properties which can significantly improve efficiency of the heat transfer processes. We examined the effect of morphology of carbon-based nanomaterials on thermal conductivity, density and viscosity of INFs. The geometry and properties of nanoparticle-liquid interface were determined by transmission electron cryomicroscopy (cryo-TEM). The 1-butyl-1-methylpirrolidinium bis(trifluoromethyl sulfonyl)imide [BMPYR][NTf<sub>2</sub>] and 1-ethyl-3-methylimidazolium thiocyanate [EMIM] [SCN] as well as Nanocyl NC7000<sup>™</sup> MWCNTs and in-house 16h MWCNTs (diameter of 60-80 nm, length of 770 µm) were selected as INFs components. The modification of [BMPYR][NTf<sub>2</sub>] and [EMIM][SCN] by 1 wt% Nanocyl MWCNTs resulted in an increase of thermal conductivity by 11% and 14%, respectively. Significant thermal conductivity enhancement of 41% and 44% was observed for INFs composed of 1 wt% in-house MWCNTs +[BMPYR][NTf<sub>2</sub>] and +[EMIM][SCN], respectively. Thermal features of INFs showed a remarkable enhancement with increasing aspect ratio of dispersed MWCNTs. The obtained results show that ionanofluids can be non-Newtonian, viscoelastic with shear thinning and thixotropic behavior.

#### ACKNOWLEDGES

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#### APTES FUNCTIONALIZED MAGNETIC DIATOMITES FOR ENDOSULFAN REMOVAL FROM SOLUTIONS: CHARACTERIZATION, THERMODYNAMICS, AND ISOTHERM STUDIES

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Because pesticides are one of the most critical environmental pollutants, their removal from environmental water samples is a matter of interest among the research community. In this study, (3-aminopropyl)triethoxysilane (APTES) functionalized magnetic diatomite particles were synthesized and used to remove endosulfan, chosen as a model pesticide, from liquid systems. Fourier transform-infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), energy dispersive X-ray (EDX), electron spin resonance (ESR), and surface area measurements via Brunauer-Emmett-Teller (BET) model were utilized for the characterizing the physicochemical properties of the particles synthesized. After characterization studies, the adsorption capacity, approximately 97.2 mg endosulfan/g particle was achieved with APTES functionalized magnetic diatomite (m-DE-APTES) particles. Linear and non-linear adsorption isotherms were studied, and thermodynamic parameters were calculated. In the calculations, it was seen that adsorption was more suitable to the Langmuir model, and the adsorption process took place spontaneously. In conclusion, the modified diatomite particles could be classified as a novel alternative adsorbent for pesticides removal from liquid systems.

**KEYWORDS:** Silane; magnetic diatomite; endosulfan; removal; adsorption isotherms; thermodynamic.

#### THE SIZE EFFECT OF CARBON NANOFILLERS ON THE THERMAL CONDUCTIVITY OF HDPE-BASED HYBRID NANOCOMPOSITES

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In this study, two different dimensions of multiwall carbon nanotubes (MWCNTs)<sup>1,2</sup> and three different dimensions of graphene nanoplatelets (GnPs)<sup>3</sup> were used to investigate the size effect on the thermal conductivity of highdensity polyethylene (HDPE)-based hybrid nanocomposites with 5 wt.% total nanofillers loading at six different weight ratios of GnPs/MWCNTs (5/0, 4/1, 3/2, 2/3, 1/4 and 0/5). All samples were prepared by using melt mixing, followed by compression molding. Measurements of density, specific heat, and thermal diffusivity infrared photothermal radiometry technique (IR-PTR)<sup>4</sup> were performed and effective thermal conductivities of nanocomposites were calculated using these values. The IR-PTR has proven its effectiveness to thermally characterize several categories of materials through a non-destructive approach. The results show that the size and weight ratio of carbon-based nanofillers play a critical role in determining the thermal conductivity. The highest thermal conductivity (0.504 W/mK) is achieved by the nanocomposite containing GnPs with the largest lateral size and MWCNTs with a higher aspect ratio at a 3/2 weight ratio at 5wt.% total filler content. In terms of GnPs/MWCNTs weight ratio, all hybrid nanocomposites exhibit a marginal thermal conductivity enhancement. In addition, the majority of hybrid system of GnPs and MWCNTs does not provide synergic improvement on the thermal conductivity, but only obeyed the mixture rule. In hybrid nanocomposites, MWCNTs with high aspect ratio are more beneficial than with smaller ones to from effective thermally conducting network and achieve higher thermal conductivity. As comparing GnPs with same diameter, thicker one shows better performance than thinner one. The combination of GnPs with large diameter and MWCNTs with high aspect ratio is more effective to achieve greater thermal conductivity. It is followed by the combination of GnPs with small diameter, but same thickness and the same MWCNTs.

Keywords: Polymer nanocomposites, carbon-based nanofillers, thermal conductivity, electrical conductivity

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#### PHASE EQUILIBRIUM STUDIES OF AQUEOUS BIPHASIC SYSTEMS INVOLVING IONIC LIQUIDS AND ZWITTERIONS

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Growing emphasis on development of sustainable and eco-friendly methods led to the search of alternative solvents for sseparation and purification processes. Systems consisting of aqueous ionic liquids (ILs) and zwitterions (Zls) as in IL- and Zl- based aqueous biphasic systems (ABS) have received immense attention due to their applications in development of novel, sustainable and efficient separation processes. The distinct properties of ILs like tunability of structure, solubility for compounds of wide polarity etc support their usage in the ABS as one of the constituents with combination of either inorganic, organic salts, carbohydrates, alcohols, amino acids etc., Zwitterions (Zls) are similar to ILs with positive and negative charge being present on same structure.

Proposed talk will focus on designing ABS by using ILs and ZIs with potassium salts and their systematic phase behaviour and evaluation of their ability to employ them in separation and extraction systems along with the detailed analysis on effect of various factors like temperature, pH, ions etc. The range of compounds studied includes tetrabutylammonium carboxylate based ILs, amino acid based ILs, and ZIs as components of ABS. The systematic analysis of ILs and ZIs' structure influence on ABS formation was performed followed by application of these systems for partitioning of group of bioactive compounds including amino acids, alkaloids and phenolic compounds. Studied ILs and ZIs based ABS were found to be capable of single step extraction of biomolecules. These studies provided deeper understanding of ABS formation and factors ruling the partition of biomolecules like hydrophobic effects and other relevant specific interactions. The derived knowledge aids in further advancement in terms of developing integrated extraction and separation platform, recycling and reuse of ILs etc.

#### USE OF FURAN-RING CONTAINING SCHIFF BASE COUPLED WITH SILICA NANOPARTICLES FOR SAND CONSOLIDATION PROCESS

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One of the most difficult problem to solve in the oil-gas industry is the control of sand production together with oil and gas. This issue can lead to the damage of the equipment and decrease the well productivity, and in consequence even lead to its shut-down due to high economical costs. There are various ways to prevent sand production: maintenance and workover, rate exclusion, selective completion practices, mechanical and chemical methods [1].

Chemical methods include the use of different sand consolidation agents and complex chemical systems. The application of resins, modified with certain nanoparticles, or together with surfactants, both suitable for the formation parameters, is considered an effective and perspective way for the consolidation of loose sand formations [2]. During creation of chemical system for sand consolidation many factors should be taken into account, such as effects of chemical composition, possible interaction of components, curing time, temperature, pressure, compressive strength and retained permeability of the consolidated sand. Sand consolidation process should not highly affect the permeability, because it will lead to the non-efficient production of hydrocarbons. Also the important role plays rate control, the geological structure and composition of soil, eco-friendliness [3].

In this study were performed a synthesis of furan-ring containing Schiff base on the basis of 2, 2'-(ethane-1,2diylbis(oxy))diethanamine and furfuryl alcohol and synthesis of silica nanoparticles by sol-gel method. Further was investigated their effect on sand consolidation process as components of chemical complex system. The silica nanoparticles play a role of coupling agent in this complex. Furan-ring containing Schiff base is used as a hardener.

Received nanoparticles were studied by SEM, TEM microscopy, EDS, XRD powder diffraction, UV-Vis and FT-IR spectroscopy. Synthesized furan-ring containing Schiff base was studied by 1H, 13C NMR, UV-Vis and FTIR-spectroscopy. The ability of these components to consolidate the sand was investigated in laboratory.

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#### UNCHARTED TERRITORY: PARTIALLY-SOLUBLE BINARY LIQUID ABOVE THE DIFFUSIONAL SPINODAL

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In recent years, physicists have been trying to solve problems connected with the enhancement of heat transfer. It goes without saying that modern devices require a certain temperature regime for stable work and the highest performance. Miniaturising integrated circuits tendency leads to complication of this task. One of the current approaches to this problem is to search for partially-soluble additives to the liquid heat carrier combined with an optimisation of the thermal conditions in which these additives provide a significant effect.

In this report, investigation of heat transfer in short-lived states of initially-stable binary solution with the so-called lower critical solution temperature (LCST) was carried out by the authors via the pulse heating method of a wire probe immersed in solution. This method allows to control the heating power directly during the pulse, as well as to record the corresponding response function over the heating range. Based on the primary data of the experiment (voltage drop across the probe and voltage drop across standard resistor, converted to the current in the probe circuit) the evolution of the mass-average temperature of the probe T(t) at a strictly specified heating power P(t), heat flux density through the probe surface during the pulse q(t) and, finally, heat transfer coefficient  $k(t) = q(t) \cdot [\Delta T(t)]^{-1}$  were calculated. These variables comprise the principal heat transfer characteristics in experiments with short-term powerful heat release.

An aqueous solution of polypropylene glycol PPG-425 was selected as the object of the study. In the course of the experiment, the solution was transferred consequently above the liquid-liquid equilibrium line and, finally, above the diffusional spinodal. In this work it will be shown that spinodal decomposition activates convective heat transfer mode, which brings on increasing of the energy transferred from the probe to the substance in comparison with pure water. This result can serve as a practical basis for the search of a new generation of coolants for processes involving powerful local heat generation.

**KEYWORDS:** spinodal decomposition, lower critical solution temperature, aqueous solution, PPG-425.

#### ACKNOWLEDGEMENTS

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#### **CO2 CAPTURE AND UTILISATION IN IONIC LIQUIDS**

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The CO<sub>2</sub> solubility in a variety of ionic liquids (ILs) has been widely reported in the literature showing that their tunability allows them to on demand chemically absorb/desorb over equimolar amounts of CO<sub>2</sub>. This high CO<sub>2</sub> capacity, paired with a low vapor pressure and increased thermal stability, means that they have been proposed as a suitable alternative to the aqueous amine solvents currently used in industrial CO<sub>2</sub> capture plants. ILs have the potential to overcome the disadvantages of volatility, corrosion, and the high energy penalty associated with synthesizing and regenerating MEA. For a sorbent to be used in a separation process it must also be able to withstand poisoning from impurities within the feed stream such as SO<sub>2</sub>, NOx and water. In this talk, the use of superbase ILs for the capture and utilisation of CO<sub>2</sub> will be presented. In particular, the competitive adsorption of flue gas impurities on the sorption of CO<sub>2</sub> will be discussed. In addition, the ability of the superbase ionic liquids to activate the CO<sub>2</sub> for electrochemical reduction will be shown in order to demonstrate the conversion of CO<sub>2</sub> to formate at low applied overpotentials.

#### ENERGY INTERACTION OF VERTICAL AXIS WIND TURBINES WORKING IN PAIRS: A CASE STUDY AT A SEMI-COMPLEX SITE

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Due to the rapidly developed wind turbine technology, rotor swept areas and hub heights of horizontal axis wind turbines (HAWT) are increasing. As a result of the development in the wind industry, each HAWT requires more space between each other to decrease overall wake losses in wind power plants (WPPs) which necessarily increases the land necessity for WPPs. Each HAWT must be spaced 4-6 rotor diameters away in the cross-wind direction and 8 - 10 rotor diameters away in the down-wind direction to its neighbouring HAWT for minimizing wake effects and maximizing WPP performance. Required WPP land sizes are increasing with the increase of each individual turbine power and it ends up with the 3 - 5 W power output for each meter square of WPP site for HAWTs. It is known that footprint-power-density can be increased dramatically by using vertical axis wind turbines (VAWTs) working in groups and pairs instead of HAWTs. In this study, we present an investigation of energy interaction of VAWTs working in pairs as a case study in a near-shore site located in Izmir City of Turkey by the following suggestions of IEC 61400-12-1:2017 standard. Site characteristics are defined by employing more than a year-long wind measurement data set from the same site by using a meteorological measurement station that includes a cup anemometer, a wind vane, a temperature & humidity sensor, a pressure sensor and a data logger. Besides. Darrieus type VATWs, each having 3.2m rotor diameter. 2m rotor height and 0.5 kW output power, are used for on-site performance measurements. The performance experiment of the stand-alone WAWT is repeated by adding second identical VAWT unit within a specified distance to investigate the energy interaction of VAWTs working in pairs. Until now, results show that test site has 5.6 m/s mean wind speed and 1.2 m/s mean turbulence intensity at 7.15 m height. This relatively turbulenced, near-shore site promises a wide range of wind speed with a different rate of turbulence intensity during the experiments. The preliminary results are presented in this study andit is expected to receive important results for a better understanding of the wake effect of stand-alone VAWT and the energy interaction of VAWTs working in pairs by the results of ongoing experiments.

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## THE EFFECT OF PRESSURE ON THE HEAT TRANSFER IN SUPERHEATED PARTIALLY-SOLUBLE BINARY LIQUID

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The processes of high-power heat release in fluids are characteristic of the modern engineering. As applied to liquid hydrocarbons, such processes are observed in friction units with oil lubrication, in the cycles of preparation and combustion of fuel in engines and rocket installations. As a rule, hydrocarbons in technical applications are a part of a multicomponent working fluid. Water and its vapor are one of the ubiquitous working fluid components disturbing technologists.

The present investigation is devoted to the characteristic features in the behavior of saturated hydrocarbons with micro-admixtures of water under conditions of a high-power local heat release in initially stable solution. The main task was to clarify the effect of water traces on the intensity of unsteady heat transfer in a wide temperature range and pressure range, including temperatures above the liquid-vapor equilibrium temperature for the components. The objects of study were *n*-hexane, *n*-decane and *n*-hexadecane.

For the specific mode of pulse heating of a probe immersed in a test liquid (saturated hydrocarbon), the effect of enhancement of the heat transfer through the probe surface has been revealed [1]. The effect is caused by the addition of a small amount of water to the hydrocarbon and manifests itself in the course of approaching the temperature of spontaneous boiling-up at rather low values of the reduced pressure  $\pi < 0.2$ , where  $\pi = p/p_{c}$ ,  $p_{c}$  is the critical pressure of the hydrocarbon. The water content was varied from 5 ppm (initial sample) to 35 ppm (watered sample). The length of the heating pulse, depending on conditions of the experiment, was varied from 5 to 20 ms. On the basis of the experimental results, we have proposed a hypothesis that when the liquid is superheated, the water contained in saturated hydrocarbons in the form of clusters generates its "own" centres of vapor phase nucleation.

#### ACKNOWLEDGEMENTS

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## DIELECTRIC PROPERTIES OF Cd<sub>1-x</sub>Fe<sub>x</sub>Te SEMIMAGNETIC SEMICONDUCTORS

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This work presents the results of experimental studies of the dielectric properties of semimagnetic semiconductors  $Cd_{1-x}Fe_xTe$  (x = 0.08). To measure the temperature dependences of the dielectric permittivity and conductivity of  $Cd_{1-x}Fe_xTe$  (sizes 0.35mm, 0.5mm, 0.2mm), silver contacts were applied to both surfaces of the sample. Capacitance and resistance were measured with E7-20 digital immitance meters (frequency 25Hz - 1MHz) at temperatures T = (115 to 465) K.

The temperature dependences of the dielectric permittivity of  $Cd_{1-x}Fe_xTe$  have been studied for different measurement frequencies for iron concentration x = 0.08 (Fig.1). It was determined that at low temperatures  $T = (165 \div 250)$  K the dielectric permittivity of the samples remains constant over the entire measured frequency range. Starting from the temperature T = 250 K, with increasing temperature, an increase in the permittivity  $\varepsilon$  is observed, and the higher the measurement frequency, the later the growth begins. The slope of the curves obtained at low frequencies up to a frequency of about 200 kHz remains constant, at frequencies above 200 kHz, an increase appears with a tendency towards saturation.

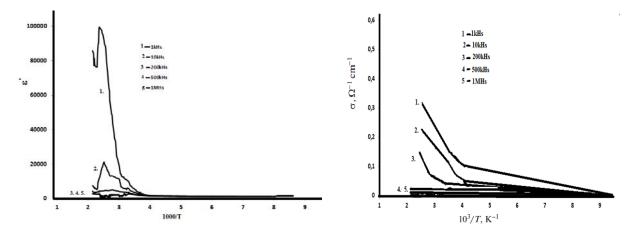


Figure 1. Temperature dependences of dielectric permittivity for  $Cd_{1-x}Fe_xTe(x=0.08)$ 

Figure 2. Temperature dependences of conductivity for  $Cd_{1-x}Fe_xTe(x=0.08)$ 

The temperature dependences of the conductivity were studied, it was found that up to a frequency of about f = 500 kHz,  $\sigma$  increases, and at a temperature of T = 250K, a sharp increase in the curves occurs (Figure 2). The slope of the curves obtained at different measurement frequencies remains constant. At frequencies f > 500 kHz, a further increase appears with a tendency towards saturation.

Comparing the results obtained for  $Cd_{1-x}Fe_xTe$  for the composition x = 0.08 with the results obtained by us in previous works for the composition x = 0.03, we can conclude that the conductivity increases with an increase in the Fe concentration in the composition.

#### ACKNOWLEDGEMENTS

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## THERMAL CONDUCTIVITY OF PHASE CHANGE MATERIALS USING THE TRANSIENT HOT WIRE TECHNIQUE

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The increasing use of energy for everyday applications and the reduce of natural resources made demanding the need for new environmentally friendly, renewable and reusable systems. Research is turning to the thermal energy storage technologies which allow the storage of thermal energy by heating or cooling a material while the same energy can be used later with a reverse procedure.

Phase change materials (PCMs) are the substances that release or absorb significant amount of energy when there is a transition from one physical state to the other. The PCMs used in thermal energy storage applications should have high latent heat and thermal conductivity. In addition, the melting temperature of the selected materials should be between the application range.

The Phase Change Materials are divided to organic, inorganic and eutectic materials with organic ones to be the most popular for many applications. The organic PCMS which studied during this work are categorized to paraffins and non-paraffins.

Even though the organic PCMs have low thermal conductivity compared to the other two types and the there is a large volume change between the phases, they have the advantage that they are quit cheap, recyclable, non-corrosive, not dangerous to use and there is an availability of PCMs within a wide temperature range suitable for different applications.

In this work the thermal conductivity measurements of Phase Change Materials (PCM) with a Single Transient Hot-Wire (THW) sensor are presented. The warm fluid in liquid phase was poured in the cell and the bottom lid screwed. The unique spring design of the bottom lid allows sample expansion and contraction, while ensuring sample is in constant contact with the THW wire during the measurements. The spring on the bottom of the cell allows thermal conductivity measurements over temperatures for fluid thermal expansion up to 15 %.

The transient hot-wire software has the advantage of the auto-detection of the power at each temperature step and measurement time only 1 s. The thermal conductivity measurements are repeatable for continuing circles of thermal conductivity measurements from high to low temperatures and then increasing to high temperatures. From the measurements the melting/solidification temperature range can be seen.

The repeatability of the measurements is better than 1 %, while the accuracy of the thermal conductivity measurements is better that 5 % for both liquid and solid phase.

KEYWORDS: Thermal Conductivity, Phase Change Materials, Sensor

## NEW MAGNETIC TOPOLOGICAL INSULATOR PHASES IN THE MnBi<sub>2</sub>Te<sub>4</sub>-SnBi<sub>2</sub>Te<sub>4</sub>-Bi<sub>2</sub>Te<sub>3</sub> SYSTEM

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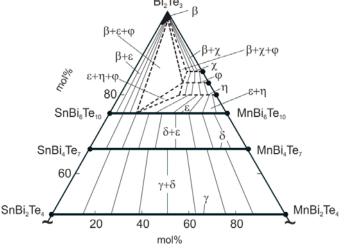
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Ternary compounds in the A-B-Te (A = Mn, Ge, Sn, Pb; B = Sb, Bi) systems have been the subject of intensive studies in the last few years because of their excellent thermoelectric and recently discovered topological insulator (TI) properties [1,2]. After  $MnBi_2Te_4$  was named the first antiferromagnetic TI [3], the search and investigation of other possible phases with similar properties intensified [4-6].

This work focuses on the investigation of solid phase equilibria in the MnBi<sub>2</sub>Te<sub>4</sub>-SnBi<sub>2</sub>Te<sub>4</sub>-Bi<sub>2</sub>Te<sub>3</sub> system in order to obtain new variable composition phases – potensial magnetic topological insulators.

Alloys of various sections of the studied system were synthesized by direct melting of pure elemental components in the evacuated (~10<sup>-2</sup> Pa) quartz ampules at 1100 K followed by quenching in icy water. Then, samples annealed at 700 K for 45 days. Resulting ingots were examined using differential thermal analysis (LINSEIS HDSC PT1600), powder X-ray diffraction (Bruker D2 PHASER) and scanning electron microscope (Tescan Vega 3 SBH) equipped with energy dispersive X-ray spectroscopy (Thermo Scientific UltraDry Compact EDS detector) techniques.

Based on powder X-ray diffraction results of annealed alloys, the phase equilibrium diagram of the MnBi<sub>2</sub>Te<sub>4</sub>-SnBi<sub>2</sub>Te<sub>4</sub>-Bi<sub>2</sub>Te<sub>3</sub> system at 300 K has been constructed (Fig.). It was established that continuous series of solid solutions are form in three section of system. namely SnBi<sub>2</sub>Te<sub>4</sub>-MnBi<sub>2</sub>Te<sub>4</sub>  $(\gamma$ -phase). SnBi<sub>4</sub>Te<sub>7</sub>-MnBi<sub>4</sub>Te<sub>7</sub> (δ-phase) and SnBi<sub>6</sub>Te<sub>10</sub>-MnBi<sub>6</sub>Te<sub>10</sub> ( $\epsilon$ -phase). Additionally, we assume that measurable homogeneity regions based on MnBi<sub>8</sub>Te<sub>13</sub> ( $\eta$ -phase), MnBi<sub>10</sub>Te<sub>16</sub> ( $\phi$ -phase) and MnBi<sub>12</sub>Te<sub>19</sub> ( $\chi$ -phase) may exist in Bi<sub>2</sub>Te<sub>3</sub> rich side. However, we are not yet able to synthesize these



phases in a pure form that is why relevant parts of the Gibbs triangle were drawn by the dashed line. Obtained novel solid solutions are of great interest as potential magnetic TI phases.

#### ACKNOWLEDGMENT

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## **DEVELOPING AND SETUP OF CONSTANT VOLUME PIEZOMETER UP TO 4000 bar**

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Current fuel injection systems for diesel engines reach pressures of approximately 1600 bar for transport systems. Future systems target even higher pressures up to 4000 bar. The possible number of injections per cycle at such extreme pressures can be expanded, while the time of one injection can be reduced. Under such high pressure conditions, however, it is necessary to know the thermophysical properties of the fuel, as they can increase up to approximately 10 times atmospheric levels. Upon injection of the fuel into the cylinder, the large depressurization of the fuel results in a significant gradient of the viscous properties of the fluid [1]. In this case, the study of the thermophysical properties of the new alternative biofuels is very important. The density, viscosity, speed of sound, and heat capacity are the main thermophysical properties for the study of such processes [2].

Such high state parameter thermophysical properties of fuels can be investigated using the newly built automatic constant volume piezometer method. The main part of the installation, designed to measure density, is a spherical, thick-walled, high-pressure piezometer measuring cell. The complete installation was planned for high pressures up to 4000 bar. The following steps were carried out during the inspection control of the piezometer: 3D and 2D determination of the inside and outside geometrical sizes and design of the piezometer; the finite element method (FEM) calculation and analysis; purchase of piezometer was constructed and tested, it was connected with tubes and setup up in the constant volume piezometer installation. To create and stabilize temperature, the piezometer was connected to the high-pressure measuring tube through the heat transfer reservoir. The installation was designed for high pressures up to 4000 bar, and so all high pressure connections were constructed to the maximum pressure, around 4000 bar.

The measured start and finish temperatures are indicated to the LabVIEW control system, and the heating of heat transfer fluid inside the heat transfer reservoir is started. Equilibrium temperatures are measured by all thermometers, and pressure readings are performed at 1-minute intervals. After stabilizing and recording the pressure within the system at each given temperature, the PC uses the Labview Program to increase temperature according to the predetermined intervals. This procedure continues up to the last measured temperature T = 473.15 K, after which the PC stops the thermostat and the measurements are complete. The measurements can be repeated many times, and can also be recorded from high to low temperature intervals. The measured pressures are then compared.

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## MEASUREMENT OF REFRIGERANT SOLUBILITY IN LUBRICANTS AT VACUUM PRESSURE USING HIDEN GRAVIMETRIC MICROBALANCES

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In refrigeration compressors, lubricants reduce friction losses and transfer heat. Viscosity, thermal conductivity, and heat capacity depend on the temperature and the solubility of the refrigerant in the lubricant. If the solubility is to be measured at vacuum pressure, potential contamination and evaporation become a challenge.

We compare the methodology of experiments with gravimetric microbalances at pressures higher and lower than ambient atmospheric pressure by means of the solubility of R-125 (Pentafluoroethane) and R-1336mzz(Z) ((Z)-1,1,1,4,4,4-Hexafluoro-2-butene) in polyol ester lubricants with viscosity grades of 32 and 68, respectively. First, we explain the handling of the gases, then the measurement procedure, and finally methods for evaluation.

The comparison shows that the handling and procedure for vacuum pressure measurements are more extensive, whereas the evaluation of measurements at high pressure can be more complex. Gravimetric microbalances are suitable for measuring binary refrigerant-lubricant systems at all pressures as long as the lubricant evaporation rate is insignificant.

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## THERMOPHYSICAL PROPERTIES OF CALCIUM NITRATE BASED TERNARY SALT MIXTURES FOR SOLAR THERMAL APPLICATIONS

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The need for clean energy has driven the solar thermal technology to its current potential. However, there is still scope for improvement especially pertaining to the Heat Transfer Fluid (HTF). Among the currently used HTFs, Solar Salt® has the highest operating temperature (~565 °C). However, the freezing point is also high (~223 °C). This limits its operation during off-peak hours. The current study focuses on the development of a ternary salt with the composition 36% Ca(NO<sub>3</sub>)<sub>2</sub> - 16% NaNO<sub>3</sub> - 48% KNO<sub>3</sub>. It was observed to have comparable decomposition temperatures as that with Solar Salt® but the freezing point was significantly lower (~142 °C), which could improve on the off-peak operation of the power plant. The current work focuses on the measurement of the melting point of the salt using cooling curve technique as well as various thermophysical properties like density and viscosity was measured. The thermal stability of the ternary salt was also measured and was found to decompose at 600 °C (more than 3% mass loss). Corrosion studies of the salt against SS304 coupons was also carried out. A comparison of various properties is shown in the Table 1 below against Solar Salt® and Hitec® salt.

Table 1: Thermophysical properties of Solar Salt compared with the new ternary salt

	Solar Salt®	Ca(NO <sub>3</sub> ) <sub>2</sub> –NaNO <sub>3</sub> –KNO <sub>3</sub>	Hitec®
Density (g/cc)	1.84 @ 400 °C	1.93 @ 400 °C	1.87 @ 400 °C
Viscosity (cP)	3.2 @ 300 °C	4.9 @ 300 °C	3.16 @ 300 °C
Corrosivity on SS304 (µm/yr.)	6-10 @ 570 °C	2.58 @ 400 °C	N.A.
Melting point (°C)	223	~130	142
Decomposition tempe- rature (°C)	600	590	535

From the values obtained it is observed that the ternary salt is a potential candidate for HTF in Solar Power Plants. Further studies related to this work is underway.

## THERMAL TRANSPORT PROPERTIES OF NANOCOMPOSITES MADE OF NANOPARTICLES EMBEDDED IN DIELECTRIC MATERIAL

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There is considerable interest in understanding heat transport in nanocomposites [1-2]. Nanocomposites with high thermal conductivity can be used to fabricate temperature-dependent nanodevices. For instance, thermal devices such as thermal diodes and thermal transistors are important devices for the heat management and control. The heat transport plays a significant role in integrated circuit chips which generate huge heat fluxes in extremely small areas. Hence, controlling heat fluxes in nanocomposites are very important for future generations of integrated circuits. Nanomaterials are also of great interest due to their potential applications as electrodes in batteries, catalysts in microreactors and in fuel cell technology. Here we present a theory of the thermal conductivity for nanocomposite made by embedding nanoparticles in a host dielectric material. We will calculate the phonon dispersion relation using the transfer matrix method in the long-range approximation, where the phonon wavelength is larger than the size of the nanoparticle. The thermal conductivity is evaluated with the Kubo formalism and the Green's function method. It is also found that the density of states, phonon velocity and thermal conductivity depends on the size of the nanoparticle, spacing between nanoparticles, and the phonon refractive index of the nanoparticle and the host material. We have also applied our theory to explain the experimental thermal conductivity data of silica-resin, alumina-resin, AIN-resin and CaO-polyethylene nanomaterials. A good agreement between theory and experiments is achieved. Our results furthermore illustrate that one can fabricate new types of nanomaterials with high and low thermal conductivity by adjusting the refractive index contrast between nanoparticles and the host material. These are very novel and interesting properties and they can be used to fabricate new types of thermal devices.

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## LATEST DEVELOPMENTS ON ANTIMICROBIAL PERFORMANCE OF THERMOPLASTIC COMPOUNDS

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An antimicrobial surface contains an antimicrobial agent that inhibits the ability of microorganisms to grow on the surface of a material. Bacteria, fungi, and algae can affect the esthetic and physical properties of a plastic by causing black spotting or discoloration, pink staining, odor and polymer degradation, fouling, etc. The most common and most important use of antimicrobial coatings has been in the healthcare setting for sterilization of medical devices to prevent hospital associated infections and also where it is needed to provide a suitable environment for many bacteria, fungi, and viruses to grow when in contact with the human body which allows for the transmission of infectious disease. The incorporation of antimicrobials or other molecules in a polymer matrix by melt processing has the advantage to use equipment commonly used to process thermoplastic materials, thus ensuring large production volumes and solventless environments. Antimicrobial polymers are produced by attaching an active antimicrobial agent on to a polymer structure. Antimicrobials used in thermoplastics have different origins such as organic and inorganic. Especially nanoparticles are used for a variety of different antimicrobial applications due to their extraordinary behavior due to their highly reactive nature. In this presentation latest developments in the research of antimicrobial polymers are given such as new classes of compounds and new production techniques.

## THERMOPLASTICS BASED COMPOSITE MATERIALS FOR ELECTROMAGNETIC SHIELDING

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Electomagnetic interference (EMI) has a significant effect on the performance of a device or system. Electomagnetic shielding is the process of reducing the dispersion of magnetic waves by using a shield made of conductive material.Reflection is the primary mechanism of EMI shielding. There are three mechanisms for EMI atenuation which are reflection, absorbtion and reflection. Reflection is the primary mechanism of EMI shielding. Metals are the most common material to be used for EMI shielding but they are expensive, heavy, hard to manifacture and prone to corrosion. Therefore conductive polymer composites due to cost effectiveness, lightweight, easy processability and applicability of different areas including EMI shielding are of great interest of both academia and industry. Polymer composites based on carbon nanotubes, carbon black, graphene, carbon fibers, metal nanoparticles, foams and magnetic nano particles have been shown to havegood EMI shielding capacity. In this presentation latest developments on the materials used for electomagnetic shielding is reviewed.

# **Flash Presentations**

## SYNTHESIS OF ORGANIC ACIDS BASED ON NAPHTHENE-PARAFFINIC HYDROCARBONS IN THE PRESENCE OF METAL-CONTAINING CATALYTIC SISTEMS

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The urgency of the problem of obtaining synthetic petrolium acids is determined by a wide area of use. Plasticizers, components of highly effective fuel and oil compositions, synergistically active reagents preventing acidic corrosion of metals, catalysts, emulsifiers, bactericides, surfactants, solvents of polymers, dyes and rubber, varnish components, antiseptic agents, additives to printing inks and anti-knock additives are obtained on the basis of them in industry. Metal  $\beta$ -diketonates are the most convenient model for studying of chelate complexes in the oxidation reaction of various substrates, however, these compounds were not used in the aerobic oxidation of petroleum naphthenic hydrocarbons [1].

The work objective is studying of aerobic oxidation process of naphthenic hydrocarbons isolated from the petroleum fraction, both in the presence of transition metals  $\beta$ -diketonates and also their modified forms. A diesel distillate (fraction at 216-350°C), isolated from Azerbaijani petroleums mixtures was selected as the object of the studies. The diesel distillate was previously dearomatized. The dearomatized petroleum fraction was oxidized in a bubble-type flow reactor equipped. The reaction was carried out at temperature of 125-140°C and air flow rate of 0.03 m3 / kg·h.

The reaction was studied in the presence of complexes of diketonates of various metals with 2,4-dinitrophenylhydrazine (DNPhH) for determination of the effect of electron-donor complexing additives on the selectivity of oxidation and the yield of SPA and OSPA (table1).

Table 1.Test results of 2,4-dinitrophenyl derivatives of β-diketonates of transition metals in the process of liquidphase oxidation of the naphthene-isoparaffinic fraction (t = 125-130 °C, air flow rate 0.3 m<sup>3</sup>/kg·h, reaction time 5 h)

	A.n. of the	SPA		OSPA		SPA+OSPA
Catalyst (amount) 0,2%	oxidate, mgƘOH/g	A.n., mgKOH/g	Yield,%	A.n., mgKOH/g	Yield, %	Yield,%
	77	153	18	143	16	34
I	51,8	139,4	13,2	135,37	10	23,2
	52,5	146,47	15	105	11	26

**Note:** I-The complex of  $\beta$  –diketonate of Mn with 2,4-DNPh, II-The complex of  $\beta$  –diketonate of Cr with 2,4-DNPhH, III-The complex of  $\beta$  –diketonate of Co with 2,4-DNPhH

Thus, as a result of the studies, it was found that addition of nitroradicals into the ligand environment of  $\beta$  - diketonates of transition metals causes an increase in the rate and selectivity of the reaction, and also helps to decrease the process temperature by oxygenated air oxidation of naphthene-paraffin concentrate to produce synthetic and oxysynthetic acids. The yield of petroleum acids mixture amounts to 40.1% by the joint use of modified  $\beta$ -diketonates of Cr and Co.

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## LIQUID-PHASE AEROBIC OXIDATION OF N-PENTADECANE IN THE PRESENCE OF AN ULTRASOUND-TREATED CR CONTAINING CATALYST

#### Vagif ABBASOV, Aygun ALIYEVA, Ulviyya KARIMOVA

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Catalysts of various structures are used to intensify technological processes, and various physical effects are used to enhance their activity — vibration, magnetic treatment, ionizing radiation, visible light, electromagnetic waves, etc. It seemed interesting to use ultrasonic waves (UW) to activate metal salts of variable valency as catalyst (Cr naphthenate) for aerobic liquid-phase oxidation of a model hydrocarbon - n-pentadecane, where the research results exceeded expectations.

Results of oxidation of n-pentadecane in the presence of Cr naphthenate (Cr naph) catalyst  $(T = 135-140^{\circ}C, \text{ amount of air} - 20 \text{ atm. at } \tau=6 \text{ hours})$ 

Catalyst	Amount of	UW,	Reaction	Induction	A.n. of	CFA		HCFA	
	catalyst, wt %	min	time, hour	period, hour	oxidate, mq KOH/q	Yield, %	A.n. mqKOH/q	Yield, %	A.n. mqKOH/q
-	-	-	12.0	3.0	42.0	1.1	-	0.4	-
Cr naph	0.1	-	12.0	2.0	56.0	4.0	146.1	2.0	150.0
Cr naph	0.1	1.0	6.0	1.5	66.77	16.7	149.3	8.33	156.0

CFA-carboxylic fatty acids, HCFA-hydroxycarboxylic fatty acids, A.n.-acid number, UW- ultrasonic waves

The research results show that the oxidation of the substrate in the auto-oxidation mode and with the catalyst takes 12 hours, but with a small yield of reaction products. And in the case of using a catalyst treated with ultrasonic testing, the process starts shortening the induction period, which also coincides with the change in the valence state of the metal in the catalyst ( $Cr^{2+}$ -  $Cr^{3+}$ ). This is because the reaction between the reaction molecule (valence - saturated particle) and the metal of variable valency of the catalyst with the transition of one electron should inevitably lead to the formation of a free radical or atom. For example, in the reaction of a divalent metal  $M^{2+}$  with a molecule A: B, a trivalent metal and a free radical or atom are formed:

$$M^{2+} + A:B \rightarrow M^{3+} + B^{-} + A^{-} (or A^{-} + B^{-}).$$

The same thing happens when the metal reverses from a trivalent state to a divalent state:

$$M^{3+} + A:B \rightarrow M^{2+} + B^{\bullet} + A^{+} (or A^{\bullet} + B^{+}).$$

Summarizing the conclusions of the table, it is observed that with the use of ultrasonic testing of the effect on the catalyst, the reaction time also decreases by 2 times, i.e., ultrasonic testing contributes to the activation of the catalyst. A decrease in the induction period by 2 times is also observed. As a result of research, there is a sharp jump in the increase in the yield of reaction products by 8 times, compared with autocatalysis.

## ULTRASOUND IN THE OXIDATION OF PARAFFINS CATALYSED BY METAL NAPHTHENE

#### Vagif ABBASOV, Aygun ALIYEVA, Ulviyya KARIMOVA

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Hydroperoxides, which are the primary molecular products of hydrocarbon oxidation reactions, play an important role in the branching process. The reactions between the hydroperoxides and the catalyst serve as powerful impulses for the formation of free radicals. The mechanism of decomposition of peroxides by cations of variable valency was first proposed by F. Haber and J. Weiss [1], who suggested that the process proceeds with the decomposition of hydroperxides under the influence of ferrous ions. Initially, Fe<sup>2+</sup> ions react with hydroperoxide to form radicals, and then the metal transitions from the divalent state to the trivalent state:

 $Fe^{2+} + ROOH \rightarrow Fe^{3+} + OH^{-} + RO^{-}$ 

Hydroperoxide, in the presence of a catalyst, decomposes with a significantly lower activation energy - 10-12 kcal/mol, versus 30-40 kcal/mol - in the absence of a catalyst. The reaction between the hydroperoxide and the catalyst proceeds with the formation of a free radical and a new polar bond (rather than an ion, as in an aqueous solution), for example, in the case of metal naphthenate of variable valency M (Naft) 2 (M-metal), the formation of new active centers can be represented in the following way:

 $\begin{array}{l} M(Naft)_2 + ROOH \rightarrow (Naft)_2MOH + RO \\ (Naft)_2M OH + ROOH \rightarrow M(Naft)_2 + ROO \\ \cdot + H_2O \end{array}$ 

The resulting radical initiates chain decomposition of the substrate. The acceleration of the formation of oxygencontaining groups is possible additionally due to the introduction of ultrasonic cavitation into the system, which was carried out on a Hielscher (Ultrasound Technology, Germany) UP200St cavitation unit (operating frequency-26 kHz). A glass sanatrode brand s26d40 ("Hielscher"), with a diameter of 40 mm and an amplitude equal to 9  $\mu$ m. As a result of the experiments, on the oxidation of paraffins in the presence of a catalyst - a metal of naphthenate, using ultrasound, it was found that ultrasound contributes powerfully accelerate the process of activation of the catalyst in the oxidation of hydrocarbons.

Nevertheless, the kinetics and mechanism of the catalyzed decomposition of hydroperoxides in hydrocarbon solutions are still poorly understood and require additional research.

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## EPOXIDATION OF SOYBEAN OIL WITH HYDROGEN PEROXIDE IN THE PRESENCE OF ORGANIC ACID

#### Vagif ABBASOV, Leylufar ALIYEVA, <u>Nigar RZAYEVA</u>, Leyla NASIBOVA

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The high reactivity of the epoxy groups in the composition of vegetable oils creates the conditions for obtaining on their basis a wide range of chemicals, for example, polyols, glycols, carbonyl compounds, lubricants, plasticizers for polymers, adhesives, etc. This makes it possible to create new technologies of "green chemistry" aimed at replacing petroleum products with renewable bioresources, due to which both the demand for vegetable oils and their production are steadily growing over the years [ref.]. Soybean oil is of particular interest for the epoxidation process, as it contains a significant amount of mono- and polyunsaturated fatty acids and is affordable both in price and in production volumes.

The epoxidation of soybean oil with formic acid and hydrogen peroxide has been studied using sulfuric or phosphoric acids as a catalyst. It was shown that the rate of the epoxidation reaction is mainly strongly affected by temperature, and the concentration of catalyst at the initial stages. The developed two-phase kinetic model takes into account all ongoing reactions in the aqueous phase (oxidation of formic acid to formic acid and decomposition of hydrogen peroxide), in the oil phase (epoxidation), and at the water-oil interface (reaction of the opening of the epoxy ring), respectively.

A simplified diagram of the equilibrium distribution of compounds and ongoing reactions in the aqueous and organic phases is shown in Figure 1.

Organic phase	Formic Acid + Epoxidized Soybean Oil ← Performic Acid + Soybean oil
Water phase	Formic Acid + Hydrogen Peroxide $\rightarrow$ Performic Acid + Water

Figure 1. A simplified scheme of the equilibrium distribution of the proceeding reactions in the aqueous and organic phases.

In contrast to the well-known literature, we have shown that the rate of the epoxidation reaction that occurs in the oil phase is about five times lower than the rate of the reaction of oxidation of formic acid into formic acid, therefore, the determining reaction is not the rate of reaction of oxidation of formic acid, but the rate of epoxidation reaction.

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## THERMOPHYSICAL PROPERTIES OF IONIC LIQUIDS

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lonic liquids (ILs) are liquid salts at the ambient temperatures. They are ideal solvents for green chemistry, have negligible vapor pressure, non-flammable, low melting point, high solvating capacity, low compressibility, high ionic conductivity, high thermal, mechanical and electrochemical stability etc., which make them attractive for practical applications. In order for design and developing reliable predictive models and to understand the nature of molecular interactions in liquid mixtures and to apply ILs in industry, the basic thermodynamic properties (density, viscosity, heat capacity, compressibility, thermal expansion coefficient etc.) are required

During the last years, we investigated the thermophysical properties of various ILs at T = (273.15 to 413.15) K temperatures and pressures up to p = 140 MPa with an estimated experimental relative combined standard uncertainty of  $\Delta p/p = \pm (0.01 \text{ to } 0.08) \%$  in density, which were investigated using a Anton-Paar DMA HPM vibration-tube densimeter [1-4]. The heat capacities at ambient pressure  $c_p(p_0, T)/\text{J·kg}^{-1}\cdot\text{K}^{-1}$  and various temperatures were measured using the differential scanning calorimeter Pyris 1.

An empiric equation of state for fitting of the  $(p,\rho,T)$  data of ILs has been developed as a function of pressure and temperature. The equation together with the heat capacity values was used for the calculation of the thermophysical properties of ILs, such as isothermal compressibility  $\kappa_T(p,T)/MPa^{-1}$ , isobaric thermal expansibility  $\alpha_p(p,T)/K^{-1}$ , thermal pressure coefficient  $\gamma(p,T)/MPa\cdotK^{-1}$ , internal pressure  $p_{int}(p,T)/MPa$ , specific heat capacities  $c_p(\rho,T)/J\cdot kg^{-1}\cdot K^{-1}$  and  $c_v(\rho,T)/J\cdot kg^{-1}\cdot K^{-1}$ , speed of sound  $u(\rho,T)/m\cdot s^{-1}$ , isentropic expansibilities  $\kappa_s(\rho,T)$  at high pressures and temperatures, in which the  $(p,\rho,T)$  data of ILs were measured.

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## AEROBIC OXIDATION OF NAPHTHENE-PARAFFINIC HYDROCARBONS IN THE CATALYTIC PRESENCE OF $\gamma$ -AI\_2O\_3 MODIFIED BY TRANSITION METALS

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Conversion of hydrocarbons separated from petroleum into valuable oxygen products is one of the actual problems in petrochemical synthesis. Oxidative conversion of petroleum hydrocarbons to oxygen compounds is one of the most efficient methods of natural hydrocarbons processing [1]. The main goal of the studies is carrying out the oxidation process in the direction of obtaining synthetic petroleum- and oxyacids (SPA and OPA) with high yield selectively, because SPA and OPA are considered as the most demanded products in petrochemical synthesis. The fraction of Azerbaijani petroleums mixture boiling at 190-330°C has been taken as a raw material for the research [2]. The fraction has been dearomatized before the oxidation process and aromatic hydrocarbons has amounted to ~1% in the fraction after the process (by sulphonation method). Dearomatized diesel fraction has been oxidized in liquid phase by atmospheric oxygen in the presence of catalytic systems with transition metals (Cr, Co, Mn) placed on nano-sized  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> by CVD method. The oxidation process has been carried out in a barbotage unit with air flow of 300 l/kg·h, the catalyst amount according to the raw material 0.2% mas., at 135-140 °C for 5 h. Nano  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> has been synthesized on sol-gel method. The results of aerobic oxidation process of naphthene-paraffinic hydrocarbons in liquid phase in 20 % mas. in the presence of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> modified by Mn-, Cr-, Co- salts are set into the table.

	Oxidate		Obtained products						
	UXIC	Jale	SF	PA	O	PA	ł,	T	
Catalyst, 0.2% mas.	A. n., mgKOH/g	Yield, %	A. n., mgKOH/g	Yield, %	A. n., mgKOH/g	Yield, %	SPA+OPA %	Unsoaped part, %	
C-1	50	98.1	132	18.54	112.93	15.5	34.04	65.96	
C-2	53.1	98.2	135.97	17.2	121.42	15	32.2	67.8	
C-3	56.73	96	118	18.5	109.57	15.2	33.7	66.3	
D-1	62	98	125.8	25.2	100.8	15.4	40.6	59.4	
D-2	48	98.4	132.76	22.55	120.57	16.57	39.12	60.88	
D-3	53.6	97	128.2	23	118	15	38	62	

**Note:** C is nano  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> obtained in the presence of MEA as a stabilizer, and D– in the presence of DEA as a stabilizer; C-1, C-2, C-3 are C modifications with Mn-, Cr and Co-salts correspondingly, and D-1, D-2, D-3 are of D, correspondingly.

As is evident from the table, catalytic activities of the catalysts obtained from DEA are higher than the catalysts obtained from MEA.

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## INVESTIGATION OF NITROGEN DERIVATIVES OF SYNTHETIC PETROLEUM ACIDS AS AN ADDITIVE TO ROAD BITUMEN

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Bitumen is a black sticky material natural derived from the fractional distillation of crude oil, and is particularly suitable as a binder for road construction. Bitumen (asphalt cement) is the most common petroleum product used in road construction industry thanks to its high adhesive and waterproofing power. The term "asphalt mixture" is a combination of mineral aggregate, bitumen, and some other inorganic and organic additives. The requirement on road bitum during the pavement consumption demands resistance to relative motion at high temperature and elasticity of asphalt at low temperature. In order to enhance the gravel bonding ability, i.e. adhesion ability many adhesion additives are used [1]. In this purpose cationactive surfactants – amidoamines, imidazolines, amine compounds and their salts are mostly used. The data of the synthesis of amidoamines obtained in the result of reaction of synthetic petroleum acids (SPA) synthesized in liquid phase by the catalytic oxidation of naphthene-paraffin hydrocarbons extracted from Azerbaijani oils mixture (fr. 185-330 °C) and polyethylenepolyamines (PEPA) in molar ratio of (1:1-6:1) are presented in the abstract. The studies have been conducted by adding the synthesized amidoamines in different percentage amount (0,4 and 0,6%) to road bitumen as an additive (table).

Adding the synthesized additives	Softeni	Needle	Extensibility	Brittleness	Adhesion
to road bitumen, imidazolines	ng	penetration	, cm	temperature, °C	
	point,	depth, at	25°C	-	with points
	°C	25°C			
		in amount 0,4	.%		
Road bitumen	48	48	75	-18	3
SPA:PEPA in molar ratio of 1:1	50.2	44	50,6	-19	1
SPA:PEPA in molar ratio of 3:1	46.3	51	70	-22	1
		in amount of 0,	6%		
SPA:PEPA in molar ratio of 1:1	47.5	49	33	-23	1
SPA:PEPA in molar ratio of 3:1	47.5	50	>100	-26	1

Table 1. Quality indicators by amidoamines addition in amounts of 0,4% and 0,6% synthesized on the bases of SPA and PEPA to road bitumen

It has been established that adding the synthesized amidoamines in small amount to road bitumen changes adhesion of bitumen from 3 points to 1 point. If take in molar ratio of SNT:PEPA = 3:1, obtained amidoamine relatively improves the consumption properties of bitumen more than other amines. Thus, when this additive is added in 0,4% to bitumen, at 25°C the needle penetration depth is 51 mm, extensibility 70 cm, brittle temperature is minus 22°C; but when 0,6% added, the softening point constitutes 47,5°C, at 25°C the needle penetration depth is 50 mm, extensibility >100 cm, brittle temperature is minus 26°C.

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## SOLID-PHASE EQUILIBRIA IN THE PbTe-Bi2Te3-Sb2Te3 SYSTEM

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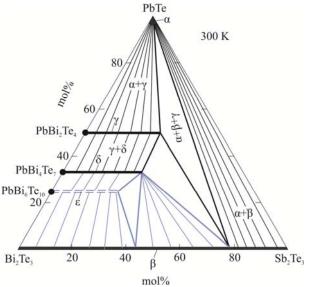
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Tetradymite-like ternary compounds as A<sup>IV</sup>B<sup>V</sup><sub>2</sub>Te<sub>4</sub>, A<sup>IV</sup>B<sup>V</sup><sub>4</sub>Te<sub>7</sub>, A<sup>IV</sup>B<sup>V</sup><sub>6</sub>Te<sub>10</sub>, etc., formed in the A<sup>IV</sup>Te-B<sup>V</sup><sub>2</sub>Te<sub>3</sub> systems (A<sup>IV</sup>-Ge, Sn, Pb; B<sup>V</sup>-Sb, Bi), are thermoelectric materials with low thermal conductivity [1]. In addition, recent studies have shown that these compounds are three-dimensional topological insulators [2-4] and are extremely promising for various applications, ranging from spintronics and quantum calculations to medicine and security systems [4,5]. One of the effective ways to develop new functional materials with controlled properties is to obtain solid solutions based on known compounds with similar properties.

This paper presents the results of studying phase equilibria in the quasi-ternary system  $PbTe-Bi_2Te_3-Sb_2Te_3$  (A) by using DTA and XRD methods. One of the boundary components of this system, namely  $PbTe-Bi_2Te_3$  is characterized by the formation of layered ternary compounds  $PbBi_2Te_4$ ,  $PbBi_4Te_7$ , and  $PbBi_6Te_{10}$ , while in the  $PbTe-Sb_2Te_3$  system, ternary compounds of this type are not formed. Therefore, the question arises about the extent of solid solutions based on these ternary compounds.

The synthesis of the starting compounds was carried out by the melting of high-purity elementary components in evacuated ( $\sim 10^{-2}$  Pa) quartz ampoules. Alloys of the system (A) were prepared by the melting of previously synthesized and identified compounds, followed by quenching from 1000 K into cold water and annealing at 800K for 500 h. and with subsequent cooling in the turn off furnace.

Based on the obtained experimental data, a diagram of solid-phase equilibria of the system at 300 K is constructed (Fig.). According to the phase diagram, this system is characterized by the formation of wide regions of solid solutions based on ternary compounds PbBi<sub>2</sub>Te<sub>4</sub> ( $\gamma$ -phase) and PbBi<sub>4</sub>Te<sub>7</sub> ( $\delta$ -phase) along the PbBi<sub>2</sub>Te<sub>4</sub>- "PbSb<sub>2</sub>Te<sub>4</sub>" and PbBi<sub>4</sub>Te<sub>7</sub>- "PbSb<sub>4</sub>Te<sub>7</sub>" sections. The extend of the  $\gamma$ -phase



is 0-55 mole % "PbSb<sub>2</sub>Te<sub>4</sub>", and the  $\delta$ -phase is 0-45 mole % "PbSb<sub>2</sub>Te<sub>7</sub>". We have also obtained preliminary data on the presence of substitutional solid solutions ( $\epsilon$ ) based on the PbBi<sub>6</sub>Te<sub>10</sub> compound. However, this phase could not be separated in a homogeneous form. It contained traces of neighboring  $\beta$ - and  $\delta$ -phases. The indicated area of the phase diagram is plotted approximately.

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## A NEW EQUATION OF STATE FOR METHANOL - WATER MIXTURE

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Water-alcohol systems are excellent solvents and are widely used in various fields of chemistry, for example, in liquid chromatography. Water-alcohol solutions are promising working fluids in absorption heat converters used in various systems for the utilization and use of low-potential energy sources. In addition, they are widely used in the food, pharmaceutical and perfumery industries, and are the basic substances for the production of nanofluids. The model for methanol-water mixture presented here is based on corresponding states theory and uses reducing parameters that are dependent on the mole fractions of the mixture constituents and critical points of the pure fluids to modify absolute values of the mixture density and temperature.

The proposed approach allows the thermodynamic properties of the mixture to be based largely on the contributions from the pure fluids. Without additional mixing functions, the model is similar to that for an ideal mixture, and only the excess values, or the departures from ideality, are required to accurately model the properties of the mixture. The model uses the Helmholtz energy as the basis for all calculations. The Helmholtz energy of the mixture is calculated as the sum of an ideal gas contribution, a real fluid contribution, and a contribution from mixing. The Helmholtz energy from the contributions of the ideal gas and the real fluid behavior is determined at the reduced density and temperature of the mixture by the use of accurate pure fluid equations of state for the methanol [1] and water [2]. Reducing parameters, dependent on the mole fractions of the constituents, are used to modify values of density and temperature for the mixture. The equation for the mixture Helmholtz energy used in this work is

$$\alpha(\delta,\tau,x) = \alpha^{0}(\rho,T,x) + \alpha^{r}(\delta,\tau,x)$$
(1)

where  $\alpha(\delta, r, x)$  is the mixture Helmholtz energy;  $\alpha^0(\rho, T, x)$  is the reduced Helmholtz energy in the ideal-gas state;  $\alpha^r(\delta, r, x)$  is the residual part of the reduced Helmholtz energy;  $\delta = \rho/\rho_r(x)$ ;  $r = T_r(x)/T$ ;  $\rho_r(x)$ ,  $T_r(x)$  is the reducing parameters suggested by Kunz and Wagner [3]

$$\frac{1}{\rho_r(x)} = \sum_{i=1}^N x_i^2 \frac{1}{\rho_{c,i}} + \sum_{i=1}^{N-1} \sum_{j=i+1}^N 2x_i x_j \beta_{v,ij} \gamma_{v,ij} \frac{x_i + x_j}{\beta_{v,ij}^2 x_i + x_j} \frac{1}{8} \left( \frac{1}{\rho_{c,i}^{1/3}} + \frac{1}{\rho_{c,i}^{1/3}} \right)^3$$
(2)

$$T_{r}(x) = \sum_{i=1}^{N} x_{i}^{2} T_{c,i} + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} 2x_{i} x_{j} \beta_{T,ij} \gamma_{T,ij} \frac{x_{i} + x_{j}}{\beta_{T,ij}^{2} x_{i} + x_{j}} (T_{c,i} \cdot T_{c,j})^{0.5}$$
(3)

where  $T_{c,i}$  and  $\rho_{c,i}$  is the critical properties of component *i*;  $x_i$  is the mole fraction of component *i*;  $\beta_{v,i}$ ,  $\gamma_v$ ,  $\beta_T$ ,  $\gamma_T$  is the binary interaction coefficients.

The ideal part can be defined by the following relation

$$\alpha^{0}(\rho,T,x) = \sum_{i=1}^{N} x_{i} \Big[ \alpha^{0}_{0i}(\rho,T) + \ln x_{i} \Big]$$
(4)

where  $\alpha_{0i}(\rho, T)$  in the ideal part of Helmholtz energy of component *i*.

The excess part can be defined by the following relation

$$\alpha^{r}(\delta,\tau,x) = \sum_{i=1}^{N} x_{i} \alpha_{0i}^{r}(\delta,\tau) + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} x_{i} x_{j} F_{ij} \alpha_{ij}^{r}(\delta,\tau)$$
(5)

where  $\alpha_{0l}(\delta, r)$  is the excess part of Helmholtz energy of component *i*;  $\alpha_{il}(\delta, r)$  is the excess function

$$\alpha_{ij}^{r}(\delta,\tau) = \sum_{k=1}^{K_{pol,ij}} N_{ij,k} \delta^{d_{ij,k}} \tau^{t_{ij,k}} + \sum_{k=K_{pol,ij}+1}^{K_{pol,ij}+K} N_{ij,k} \delta^{d_{ij,k}} \tau^{t_{ij,k}} \exp\left(-\delta^{l_{ij,k}}\right)$$
(6)

A nonlinear optimization procedure was used to develop mixture model. Optimization of the co binary interaction coefficients in Eq. 2, Eq. 3 and coefficients of Eq. 6 took place simultaneously in a nonlinear form. The uncertainties of calculated values of various properties are determined by comparisons with measured values. In addition, an array of data on the thermodynamic properties of the mixture was obtained using the Monte Carlo method. This method is supported by the statistical mechanical formalism proposed in [4]. The formalism was designed to yield any derivative of the residual Helmholtz energy from a single molecular simulation run for a given state point [5]. To control the behavior of the equation of state at high parameters, a comparison with the data of molecular simulation was also performed.

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## STUDY OF THERMAL PROPERTIES OF AgCuS by DTA METHOD

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The crystal structure and various physical properties of semiconductor AgCuS compounds have been studied for a long time there is a need for new investigations in this area using modern research methods. The thermal properties are less studied compared to other physical properties. Although the thermal expansion coefficients have been determined, the heat capacity, the free energy of the system, enthalpy have not been determined. In this work, the thermal properties of the AgCuS compounds are investigated at high temperature ranges by DTA method. Thermal parameters are determined for a different phase of structures.

AgCuS compounds were synthesized in rotary furnace from Ag and Cu metals of B5 brand and sulphur in high purity, taken in stoichiometric ratio. The synthesis was carried out in evacuated quartz ampoules. The furnace temperature was increased to melting temperature of sulphur (T = 395 K) in first step. After being kept at that temperature for t = 4-5 h, that is, after the sulfur reaction of metals (Ag and Cu), the temperature increased to the melting temperature (T = 1410 K) of the compound. After t = 4-5 h at the specified temperature, the furnace was cooled to a 60 degrees/h with the ampoule. Microstructure, X-ray phase, density determination methods (complex physical and chemical analysis methods) were used to verify the purity of the compound. Synthesized compound was annealed at T = 450 K for t = 7 h till homogenization and then studies were performed.

The crystal structure of the AgCuS compound was investigated by the X-ray diffraction method at T = 300-1000 K temperature range using D8 ADVANCE diffractometer. The diffraction data were analyzed by the Rietveld method using the FullProf program.

Thermal properties of AgCuS compound were performed by Differential Thermal Analysis method at T = 300-1300 K temperature range using Perkin Elmer STA 6000 device. The measurements were performed with 5 K/min rate. The DTA spectra obtained at the high temperature were analyzed in Origin 9 software.

The crystal structure at high temperature and thermal properties of AgCuS compound were investigated by X-ray diffraction method and DTA method, respectively. It was determined that the crystal structure of this compound corresponds to orthorhombic symmetry at normal condition and room temperature. The phase transition to high symmetry cubic phase was observed at T = 930 K temperature. According to this phase transition, endo effect was observed in the spectrum of DTA with a central peak T = 938 K. The change mechanism of enthalpy and thermal capacity around the phase transition point has been determined. It was determined that the value of the enthalpy of phase transition is equal to  $\Delta H = -6.94$  J/g. The results obtained by X-ray diffraction and DTA methods confirmed one another.

## THERMOGRAMMETRIC STUDY OF BENZYLAMINPHENOLFORMALDEHYDE OLIGOMERS

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Enhancing the characteristics of phenol-formaldehyde oligomers (PFO) by modifying them with a number of organic compounds, including nitrogen-containing compounds, is associated with their reactivity and determines the relevance of research in this direction. Thermal stability of PFOs is of great importance, since in many cases it is considered as the main indicator of the material suitability for its use. Given the foregoing, a study of the thermal characteristics of PFO functionalized by benzylamine was carried out. Resole-type PFO modified by benzylamine, obtained at a molar ratio of phenol, formaldehyde and modifier 1: 1.2: 0.2-0.4, the products of their repeated polycondensation in a solvent medium and the esterification of the latter with n-butanol were selected.

The thermal properties of the modified oligomers were studied by thermogravimetric analysis (TGA). The analyzes (TG / DTF, TF / DTA) were carried out on a "Yupiter STA449F3" thermal analyzer ("NETZSCH" company, Germany) in a nitrogen medium in the temperature range of 25-600°C, with a temperature increase rate of 10 K/min, the change in mass depending on temperature was studied.

The analysis revealed that a significant weight loss of samples up to 200 °C accompanied by endo-effects may occur due to the release of low molecular weight substances. However, it should be noted that this does not happen in the case of the initial oligomer, and dioxane and n-butanol are released for the products of its conversion, respectively. After 300 °C, destructive processes are comparatively pronounced in benzoferramine-modified PFO. Since, while this sample has a mass loss of 18.5% in the 300-600 °C temperature range, for the two subsequent products of its conversion, this indicator is 12% and 9%, respectively. Therefore, the latter are thermally more stable compared to the initial oligomer. Generally, the residual mass of all products at a temperature of - 600°C is quite high - 53-78%. Thermal decomposition proceeds in two stages for the initial oligomer, and in three stages for the products of its conversion. Significant endo-effects in the initial oligomer are expressed in the temperature range of 86-183.1°C and the area of thermal change acquires a high value - 1236  $\mu$ V / mg. Despite the multistage degradation process of the transformation products, it begins at a relatively low temperature, but occurs at a wider temperature interval compared to the initial oligomer, 53.2-203.5 °C and 47.9-193.5 °C, respectively, but the area of thermal changes is low. The difference in the peak temperatures of destruction indicates a different nature of the decomposition processes.

Thermal properties have been also studied in air. Differential thermal analysis (DTA) was carried out on a LIN-SEIS STA PT 1600 derivatograph (Germany) under atmospheric conditions with a temperature increase rate of 10 °C/min in the range up to 1000 °C. Changes in mass are recorded.

By analyzing the indicators, it can be concluded that the oligomeric macromolecules are completely oxidatively degraded within 700 °C with a residual mass of 6-10.5%. Comparison of similar indicators obtained in an inert and oxidizing medium indicates the predominance of destruction associated with oxidative processes, and not the destruction of chemical bonds. Apparently, there is not an increase observed in the thermal stability of oligomers after chemical transformations; the numbers indicate the opposite. But preliminary studies of the physicomechanical properties of composite coatings based on esterified oligomers reveal the high quality indicators of the latter in exploitation, which is likely due to a positive effect of curing processes.

## INVESTIGATION OF THE PROPERTIES OF SULFOCATIONITES BASED ON POLYMER COMPOSITION

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We have synthesized polymer-based sulfocationites. As a carcass, a polymer composition was used with the use of waste polystyrene (WPS) mechanochemically modified with a polymer mixture of chlorinated atactic polypropylene (CAPP) and polyvinyl chloride (PVC) taken in the ratio CAPP:PVC=1:1. Modification of waste polystyrene with a polymer mixture was carried out on a capillary viscometer at a temperature of 160 °C for 5 minutes. Further, based on of the obtained composition by the method of sulfonation, ion-exchange materials - sulfocationites - were synthesized.

This work is devoted to the study of the basic properties of ion exchangers, such as mechanical strength, ability to absorb, characterized by static and dynamic exchange capacity. It is determined by the number of gram-equivalents of ions absorbed by a unit of volume or mass of ionites. Therefore, a high ion exchange capacity is the main requirement for both cation and anion exchangers. Additionally, ionites should have good kinetic properties (high ion exchange rate), resistance to various acids, alkalis, as well as insolubility in water and limited swelling.

Taking into account the above, we have investigated the above-mentioned characteristics of ion-exchange materials and the results of the research are shown in Table 1.

No	Sulfocationite,% (mass) Sulfocationite based on polymer body, (%) mass WPS CAPP/PVC		Swelling Coefficient in water	SEC based on NaOH, mg-equi/g	DEC based on CaCl₂, mg-equi/g	Mechanical strength after 10 hours of shaking, %
1.	99	1	1.06	6.1	0.72	90
2.	98	2	0.98	8.8	0.99	90
3.	97	3	0.64	7.3	0.91	90
4.	96	4	0.49	6.6	0.70	90
5.	95	5	0.47	6.6	0.65	90
6.	КУ-2-8		1.03	5.1	0.65, 0.85	90
7.	BPS		0.10	2.1	0.49	80

Table 1: The main characteristics of sulfocationites obtained on the basis of the polymer composition WPS: CAPP/PVC

As can be seen from the data in the table, with an increase in the amount of CAPP/PVC mixture in the composition of the sulfocationite from 1 to 5% (mass), the swelling coefficient decreases, which is explained by the fact that CAPP and PVC are water-resistant polymers, as well as the influence of weak structuring and formation in the polymer system intermolecular interaction. This is due to the fact that during the joint processing of waste polystyrene with CAPP and PVC at temperatures above 150°C, as a result of chlorine separation and release from the CAPP and PVC macromolecule, macroradicals are formed and the components interact with the formation of a weakly cross-linked structure.

According to the table, it can be concluded that the sample of sulfocationites obtained on the basis of a polymer system containing 2% (mass) of the polymer mixture CAPP/PVC SEC and DEC have improved indicators, the values of mechanical strength also have satisfactory results in comparison with sulfocationite «KY-2».

## PREPARATION OF RUBBER COMPOSITION BASED ON BUTADIENE-NITRILE RUBBER WITH MODIFIED PHENOL-FORMALDEHYDE OLIGOMER

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Many polymers of different types are synthesized in all countries of the world, and compositions with different properties are obtained on the basis of these polymers. There is not any industry that does not use polymer composite materials. Products made of polymer-based composite materials are used in mechanical engineering, petrochemical, electrical engineering, cable industries, etc. The reason for its widespread use is due to the purchase of new composite products. One of the main ways to obtain polymer compositions with new properties is the modification of polymers. According to the latest achievements of science, it is possible to mechanically modify polymers during the processing of polymers in modern industrial technology and obtain new properties based on them.

The purpose of our research is to obtain an oil- and gasoline-resistant rubber composition based on nitrile butadiene rubber (NBR). For this purpose, a binary mixture based on phenol-formaldehyde oligomer (MPFO) modified with NBR and amine group monomer was prepared in advance.

Rheological parameters of the obtained mixture were studied. Volume consumption of alloys of the binary mixture prepared based on MPFO and NBR is 100; 120; 140; Investigated at 150 and 170 °C temperatures. It has been shown that as the amount of MPFO in a binary mixture increases at 100 and 120 °C, the volume consumption increases, indicating that MPFO plays a plasticizing role in the mixture. At 150 °C, the velocity of the 2-mass MPFO alloy increases in the mixture, while the 4- and 6-mass alloys increase the velocity of the alloy, but these two-mass fractions create maximum structuring in the NBR macromolecule. The number of alloy increases with the subsequent growth of MFFO. This suggests that at a temperature of 150 °C (4-6) MPFO is structured with NBR, which acts as a softener in the upper part of the mass. At 170 °C, the volume consumption of the alloy is nonlinear. That is, there is both destruction and structuring. That is, it is not expedient to carry out the processing at a temperature of 170 °C.

The following dependencies characterizing the rheological properties of alloys of MPFO and NBR binary mixtures under the influence of displacement deformations caused by different loads at temperatures of 100; 120; 140; 150 and 170 °C were studied:

log  $\overline{\dot{\gamma}}$  - log T; log  $\eta_{ef}$  - log T;

log  $\eta_{\rm ef}$  – the relationship between the amount of mass fraction of MFFO.

Analyzing the obtained results, it can be concluded that it is expedient to take the amount of MPFO (4-6) in these mixtures by mass.

Finally, compositions based on mixtures of butadiene-nitrile rubber (4-6) with BNF modified in bulk with MPFO in various proportions were prepared. The composition mixture is prepared on a laboratory roll at a temperature of 40-60 °C for 25-30 minutes. After storage of the prepared mixture following with the standard, it is vulcanized in a hydraulic vulcanization press at a temperature of  $153 \pm 20$  °C for 20 minutes.

Based on the results of the study, it is suggested that (4-6) the mass fraction is based on compositions based on butadiene-nitrile rubber modified with MPFO, oil-gasoline-resistant, metal-bond strength, temperature resistance, etc. products can be made.

## INVESTIGATION OF THE THERMO-OXIDATIVE DEGRADATION PROCESS OF IONITES

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By the method of sulfonation with concentrated sulfuric acid of the polymer carcass, i.e. modified composition based on waste polystyrene (WPS) and polyvinyl chloride (PVC), we synthesized ion-exchange materials [1-3]. The obtained sulfocationites in terms of their main characteristics, such as static and dynamic exchange capacity, swelling coefficient, etc. are close to industrial sulfocationite «KУ-2», which is widely used in industry for water demineralization.

Taking into account the fact that ion-exchange materials can be used in an aggressive environment, as well as at high temperatures, studies were carried out on the thermo-oxidative degradation of both the initial components and the modified composition of WPS:PVC, and ion exchangers. For this, the method of differential thermal analysis (DTA) was used and the following were determined:

- change in the mass of samples  $(\Delta m)$  depending on temperature;
- change in the mass of the test sample in time  $\left(\frac{dm}{d\tau}\right)$  depending on temperature;
- the temperature difference (∆t) during heating at a constant rate between the test sample and the standard - a thermally inert substance. Al<sub>2</sub>O<sub>3</sub> was used as an inert substance.

Differential thermal analysis of polymers was carried out in a temperature range of 20-500 °C, with a sample weighed in 100 mg, the sensitivity of galvanometers DTA - 250  $\mu$ V, DTG - 1mV. The studies were carried out in air flow in a platinum crucible; the temperature heating rate in the derivatograph furnace was 5 deg/min.

Differential thermal analysis of waste polystyrene showed that at temperatures from 100 to 220 °C, the weight loss is practically stable and amounts to 4%. At temperatures above 220-230 °C, a sharp weight loss begins. For a sample of a mechanochemically modified WPS:PVC composition, the weight loss is stable at temperatures from 50 to 275 °C and it is 3.5%. DTA of sulfocationite based on a modified mixture of WPS:PVC showed that up to a temperature of 100 °C the substance loses 3% of its weight, then the TG line goes straight and practically no decomposition occurs up to a temperature of 300 °C. Then the studied sulfocationite gradually loses weight. The sulfocationite synthesized based on the initial polystyrene has a weight loss of 48-50% at a temperature of 300 °C. Hence, we can conclude that by modifying waste polystyrene with polyvinyl chloride, a thermally more stable system is formed, as a result of which the sulfocationite synthesized on its basis is thermostable up to a temperature of 275-300 °C.

## SYNTHESIS OF SUPRAMOLECULAR ASSEMBLIES OF NICKEL NANOPARTICLES WITH NEW SCHIFF BASES

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Schiff bases, in other words, imines, are versatile molecules. They have a variety of biological applications in pharmacological areas. Some transition metal complexes were reported to have antimicrobial activities. Schiff base ligands are considered "privileged ligands" because they are easily prepared by the condensation between aldehydes and amines. Schiff base ligands are able to coordinate with many different metals, and to stabilize them in various oxidation states. The Schiff base complexes have been used in catalytic reactions and as models for biological systems. In this paper, was propose the synthsis of nickel nanoparticles, new Schiff base and their supramolecular assemblies.

$$\begin{array}{c} Br \\ Br \\ Br \\ (a) \end{array} \xrightarrow{OHC} (b) \\ (b) \end{array} \xrightarrow{OHC} (b) \\ (c) \\$$

Scheme 1. (a) Synthesis of 2.2',2"-((benzyl-1,3,5-triltris(methylene)tris(oxy)tribenzaldehyde (trialdehyde), (b) Synthesis of Schiff base

The first was synthesized trialdehyde for the synthesis of Schiff base. Trialdehyde synthesis was carried out by reaction of 1,3,5- tris(bromomethyl)benzene and salicylaldehyde [1]. The new Schiff bases are synthesized in the form shown in Scheme 1b. New Schiff bases were obtained from the reaction of synthesized trialdehyde with different aromatic amines- aniline derivatives. The synthesis of Schiff bases was carried out in the reflux for 3 hours. After the cleaning of the new Schiff bases was checked on thin-layer chromatography, their structures were confirmed by nuclear magnetic resonance spectroscopy. Also, the structure of the Schiff base was determined by FTIR, UV-vis, <sup>1</sup>H NMR, <sup>13</sup>C NMR techniques.

Nickel particles (NiNPs) in particular have emerged as a promising material because of their biological, electrical, thermal, and magnetic properties. Fundamental research on this topic has already led to the development of prototypes for the application of NiNPs for drug delivery, body motion sensing, data storage, or bioanalysis. The reaction mechanism, initial attempts were carried out according to a procedure by Wasiak et al. wherein hydrazine and sodium hydroxide was introduced to the nickel precursor [2].

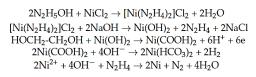
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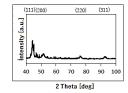
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(5)





Obtained nanoparticles are dried at ambient, further from the obtained powder is prepared the solution in distilled ethanol, to which the Schiff base is added at ratio 3:1 with further ultrasonication for 20 minutes. Samples were investigated by FTIR, XRD, TEM.

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## SYNTHESIS OF NOVEL SCHIFF BASE DERIVATIVES AND INVESTIGATION OF THEIR ANTIFUNGAL ACTIVITY AGAINST VERTICILLIUM DAHLIAE

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Schiff bases are some of the most widely used organic compounds. They are used as pigments and dyes, catalysts, intermediates in organic synthesis, and as polymer stabilisers. Schiff bases have also been shown to exhibit a broad range of biological activities, including antifungal, antibacterial, antimalarial, anti-inflammatory, antiviral, and anticancer properties. Schiff base derivatives containing a donor atom can act as good chelating agents for the transition of metal ions.

Fungal infections are not usually limited to the surface tissues; indeed, a significant increase in life-threatening systemic fungal infections has been reported. *Verticillium* belongs to the fungal class *Deuteromycetes* a group of fungi (Fig 1). Over 300 woody and herbaceous plant species are known to be susceptible to *Verticillium dahliae* including tomato, eggplant, pepper, potato, peppermint, cotton, asters, strawberries, raspberries, roses, maple, and elm. Resistant plants include all monocots, all gymnosperms, apple, crabapple, mountain ash, beech, birches, dogwood, hackberry, hawthorn, linden, honeylocust, oaks, sycamore, poplar, walnut, and willow. *Verticillium dahliae* occurs worldwide but is more important in temperate zones.

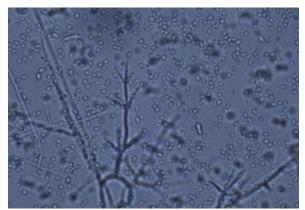


Figure 1. Microphotographs of Verticillium Dahliae

4-aminoantipyrine has an N-phenyl group and a -CH2 group on either side of a polar carbonyl group thus resembles N-substituted amides. The carbonyl group in 4- aminoantipyrine is a potential donor due to the large dipole moment (5.48 D) and strong basic characters. Since 4-aminoantipyrine has an additional potential coordination site in the amino nitrogen, it was considered worthwhile to study the complexes of this ligand. Schiff bases and metal complexes of 4-aminoantipyrine are also known for their great variety of applications in the area of catalysis and biological activity ranging from antitumour, fungicide, bactericide, anti-inflammatory and antiviral activities.

In this paper, synthesis of new Schiff base based on 4-aminoantipyrine and investigation of antifungal activity against *Vertcillium dahliae*. As shown in Fig. 2, new Schiff bases were obtained from the reaction of the synthesized 4-aminoantipyrine with different aromatic aldehydes. The structure of the Schiff base was determined by FTIR, UV-vis, <sup>1</sup>H NMR, <sup>13</sup>C NMR techniques.

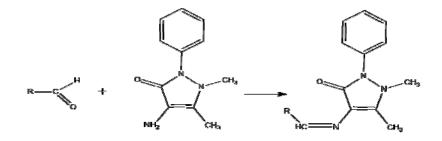


Figure 2. Scheme of synthesis of new Schiff base based on 4-aminoantipyrine

## PHASE EQUILIBRIUM IN THE RECIPROCAL SYSTEM Ag, Ge || Se, Te

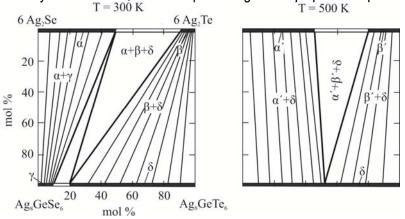
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Copper and silver chalcogenides of with germanium subgroup elements and complex phases based on them are among the promising functional materials with interesting photoelectric, optical, thermoelectric properties and ionic conductivity by cations Cu<sup>+</sup> (Ag<sup>+</sup>) [1-3]. In this work, we continued the study of quaternary systems based on silver chalcogenides [4-6] and presented new data on phase equilibria in the reciprocal system  $6Ag_2Se+Ag_8GeTe_6 \leftrightarrow 6Ag_2Te+Ag_8GeSe_6$  (A) by using DTA, XRD, and SEM methods.

The synthesis of the initial compounds was carried out by alloying high-purity elementary components in evacuated (~  $10^{-2}$  Pa) quartz ampoules. In the case of selenides, the synthesis was carried out in a two-temperature furnace. Alloys of system (A) were obtained by alloying of the starting compounds also under vacuum. All samples were annealed at 900 K for 100 h. Then, a series of alloys was held at 500 K and quenched in cold water, and the second series was additionally annealed at 400 K for 10 h.

Based on the data obtained, the projection of the liquidus surface and isothermal sections at 300 and 500 K of the phase diagram of the system (A) were constructed (Fig.). According to the data obtained in the Ag<sub>8</sub>GeSe<sub>6</sub>-Ag<sub>8</sub>GeTe<sub>6</sub> section, a continuous series of solid solutions ( $\delta$ -phase) is formed, which at 500 K form connodes with solid solutions based on the high-temperature cubic modification of the Ag<sub>2</sub>Se ( $\alpha$ '-phase) and the intermediate cubic modification of the Ag<sub>2</sub>Te ( $\beta$ '-phase). At room temperature, the homogeneity region of the  $\delta$ -phase based on Ag<sub>8</sub>GeTe<sub>6</sub> is 80 mol%. This phase forms connodes with the  $\beta$ -phase based on the low-temperature monoclinic modification Ag<sub>2</sub>Te. At this temperature, based on the low-temperature orthorhombic Ag<sub>8</sub>GeSe<sub>6</sub>, ~ 10 mol% solid solutions ( $\gamma$ -phase) are form.  $\gamma$ -phase forms connodes with  $\alpha$ -solid solutions based on the low-temperature modification of the Ag<sub>2</sub>Se. In the system at 300 K, two three-phase regions  $\alpha$ + $\beta$ + $\gamma$  and  $\alpha$ + $\gamma$ + $\delta$  are revealed.



#### ACKNOWLEDGES

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### COMPOSITIONS BASED ON EPOXY OLIGOMER MODIFIED BY FILLERS

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Epoxide oligomers (ED-16, ED-20) are widely used in the production of various materials - absorbents, coatings, adhesives and varnishes. Materials based on epoxide oligomers are used to cover or absorb different circuits and electrical conductivity in the electrical and radio industry. Stickers are used to glue the metals, rubbers, plastics, woods, ceramics. Materials based on the epoxide oligomer are starting to be accumulated during the solidification process so that the accumulation must be minimized. This remains a pressing problem.

To solve this urgent problem, the epoxide oligomer has been modified with a series of fillers. For example, it can be modified with sludge, graphene oxide and diatomite, and then other components are included. First, different amounts of polyethylene polyamine (PEPA) have been added to the ED-20 oligomer. The physical and mechanical properties of the composition have been investigated and found in various amount of PEPA in composition and then there was determined the best ration of 1:10.

Graphene Oxide used for obtaining the composition with epoxide oligomer was obtained and examined for antimicrobial properties. As Graphene Oxide has a layered structure, it has great antimicrobial properties and it is a good filler for medical technology, pharmaceutical usage. The structure of graphene oxide obtained by us for modification was investigated by the XRD method. Unlike all beneficial properties of Graphene Oxide, in the course of our experiments, it has been established and proved that an adhesive composition based on epoxy oligomer modified with diatomite has better characteristics than an adhesive composition modified with graphene oxide. We also continue these works, taking into account the change in quantitative indicators and observe a correlation.

## THERMOPHYSICAL PROPERTIES OF ALCOHOLS AND DIESEL FUEL BLENDS

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Current fuel injection systems for compression-ignition (diesel) engines reach pressures of approximately 160 MPa. Future increasing of injection pressure up to 200-300 MPa is reality. The possible number of injections per cycle at such extreme pressures can be expanded, while the time of one injection can be reduced. Under such high pressure conditions, however, it is necessary to know the thermophysical properties of the fuel, as they can increase up to approximately 10 times atmospheric levels. In this case, the study of the thermophysical properties of the new alternative biofuels is very important. The density, viscosity, speed of sound, and heat capacity are the main thermophysical properties for the study of such processes.

During the last decades, alcohols have seen increasing use as alternative fuels and have in fact been used in blends in internal combustion engines for a long time. They can be produced from biomass and from fossil fuels. Alcohols have a lower carbon content per heating value than diesel fuel, less sulphur content, and contain a significant oxygen number (higher than traditional fossil-based fuels), a much lower temperature flash point and a higher vapor formation potential in confined spaces. Alcohol fuels have a higher octane number than traditional fossil fuels. Nevertheless, alcohols have a lower cetane number, which limits the usage of neat alcohols in diesel engine as an alternative fuel. Use of cetane enhancers can improve the potential of alcohol fuel blends and is a promising fuel for diesel engines. These properties of alcohols require extra precautions, such as ensuring safe handling with the use of alcohol in alternative fuel blends. Increasing the alcohol percentage in diesel mixtures also improves volatility and viscosity at low temperatures of blend.

During the last years, the thermophysical properties of Ethanol, 1-Propanol or 1-Butanol and Diesel B0 fuel blends at T=(263.15 to 468.65) K, pressures p=(0.101 to 200) MPa and  $w_V=(0 \text{ to } 100)\%$  volume percent of alcohols were investigated in our laboratories. The density at high state parameters were studied using an Anton Paar vibration tube densimeters. Vapor pressure values were measured using the two high-accuracy static experimental installations. The dynamic viscosity were measured using an Anton Paar SVM 3000 Stabinger Viscometer and Anton Paar Rheometer MCR 302; the constant pressure specific heat capacity using the differential scanning calorimeter and the speed of sound values using the Anton Paar DSA 5000 M vibration tube densimeter and sound velocity meter.

The ultra pure propanols (w=99.995%) were purchased from Merck Schuchardt OHG, Germany and were thoroughly degassed before measurements. The Shell Global Solution DK5037 Diesel B0 fuel was used during the preparation of fuel blends. The obtained experimental results were fitted using the empiric equations.

## CRYSTALLIZATION AND PHASE TRANSITIONS OF SOLID SOLUTIONS IN THE Ag<sub>8</sub>SiS<sub>6</sub>-Ag<sub>8</sub>Ge(Sn)S<sub>6</sub> SYSTEMS

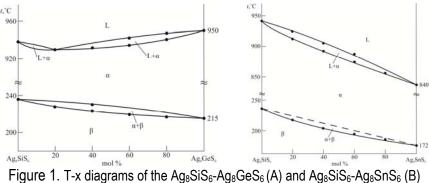
#### Sameddin ASLANLI<sup>1</sup>, <u>Geray ASHIROV<sup>2</sup></u>, Leyla MASHADIYEVA<sup>2</sup>, Isfendiyar ALVERDIYEV<sup>1</sup>, Yusif YUSIBOV<sup>1</sup>

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Silver chalcogenides with p<sup>2</sup>-elements, especially  $Ag_8A^{IV}X_6$  -type compounds are particular interest due their mixed ion-electron conductivity and are perspective for electrochemical converters of solar energy, ionselective sensors, photoelectrodes et al. [1-3]. These compounds are characterized by polymorphism. Their high-temperature superconducting modifications are isostructural and crystallize in cubic (*F*-43*m*) system, however low-temperature ones crystallize in lower symmetry. In particular, low-temperature modifications of the Ag\_8SiS\_6, Ag\_8GeS\_6 and Ag\_8SnS\_6 compounds are also isostructural and have orthorhombic structure (Sp.Gr.Pna2<sub>1</sub>). This allows us to expect the formation of continuous or wide areas of solid solutions in the systems Ag\_8SiS\_6-Ag\_8GeS\_6 (A) and Ag\_8SiS\_6-Ag\_8SnS\_6 (B).

This work is devoted to investigation of phase relations in the systems  $Ag_8SiS_6-Ag_8GeS_6$  and  $Ag_8SiS_6-Ag_8SnS_6$ and some properties of solid solutions. Starting compounds were synthesized from high-purity elements (at least 99.999 wt.% purity) in sealed silica ampoules under vacuum (10-2Pa). Synthesis was carried out in a two-zone furnace. Samples of the systems (A) and (B) were prepared by melting of the pre-synthesized compounds under vacuum also. Alloys were annealed at 900 K for about 500 h. Then one series of samples was quenched into water, and the second was additionally annealed at 400 K during 10 h.

DTA (NETZSCH DSC 404 F1 Pegasus<sup>®</sup>) and XRD (Bruker D8 ADVANCE diffractometer, Cu-K<sub> $\alpha$ </sub> radiation) were used to analyze the samples of the investigated systems. Based on experimental data, the T-x diagrams (Figure 1) are constructed.



It was shown that both systems are quasi-binary and characterized by continuous series of solid solutions between both crystal modifications. XRD analysis confirmed the formation of continuous solid solutions between both crystal modifications in the studied systems.

#### ACKNOWLEDGMENT

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## STUDY ON THE THERMODYNAMIC BEHAVIOR OF Sb-Te BINARY SYSTEMS AT THE HIGH TEMPERATURES

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Compounds with semiconductor properties are widely investigated due to their being considered as functional materials. Recently, various physical properties of these compounds have been studied under external influences such as pressure and temperature. Recently,  $Bi_2Se_3$ ,  $Bi_2Te_3$  and  $Sb_2Te_3$  binary compounds have been among the most investigated semiconductor compounds, and observation of topological isolation in these compounds has further increased interest in them. Therefore, studies of both the crystal structure and the thermal properties of these compounds is very important for explaining the various physical properties in terms of structural aspects. In this study, the  $Sb_2Te_3$  compound was synthesized, and its thermal properties were studied weeny the DTA (differential thermal analysis) method in the T = (30 - 700) °C temperature range.

The differential scanning calorimetry (DSC) measurements were carried out using the DSC3 STARe Systems manufactured by METTLER TOLEDO. The standard adiabatic calorimetry was performed in the temperature range from -150 °C to 900 °C at a heating rate of 5 °C/min in an argon atmosphere at a flow rate of 20 ml/min which had previously been calibrated with indium. The cooling process was achieved with the help of the NITRO-GEN UN 1977 REFRIGERATED LIQUID analyzer cooling system and a "digital temperature controller". The error in weight determination did not exceed 1.02% at -150 °C and 1% at 30 °C.

DSC curves consist of 4 parts in the  $50 \le T \le 700$  °C temperature range: 1)  $50 \le T \le 130$  °C: The thermal function increases with increasing temperature, 2)  $130 \le T \le 606$  °C: Wigner enthalpy interval, 3) Phase transitions at different temperatures, 4) The specific heat capacity increases with increasing temperature. The Graphical descriptions of Wigner enthalpy in the  $142 \le T \le 606$  °C temperature range and the phase transition in the  $606 \le T \le 657$  °C temperature range are shown in Fig. 1. The central peak of the Wigner enthalpy is 296 °C in the kinetics of the non-irradiated Sb<sub>2</sub>Te<sub>3</sub> compound. The energy stored in the crystal structure, in units or mass, is 14.52 J/g, and the field energy is  $72.6 \text{ }\mu\text{J}$  in the  $142 \le T \le 606 \text{ }\circ\text{C}$  temperature range. The energy of phase transition of  $626 \text{ }^\circ\text{C}$  in the  $606 \le T \le 657 \text{ }^\circ\text{C}$  temperature range is  $6.51 \text{ }\mu\text{J}$ , and the value of the activation energy is 0.07 J/mol. At temperatures up to  $700 \text{ }^\circ\text{C}$ , the value of the heat flux increases linearly with increasing temperature to  $0.36 \text{ }\mu\text{W/mg}$ .

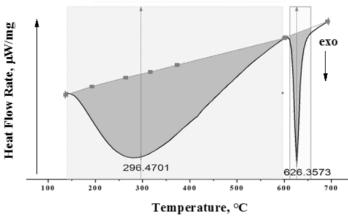


Figure 1. Wigner enthalpy and phase transition of Sb<sub>2</sub>Te<sub>3</sub>.

## THERMOPHYSICAL PROPERTIES OF GEOTHERMAL WATERS OF AZERBAIJAN

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Geothermal energy harnesses the heat energy present underneath the Earth and is generated in many places, where heat from the earth's core rises to the surface, for example where volcanoes and hot springs are present. This heat can also be exploited in by drilling down 3-5 km to reach 'hot rocks' with temperature at or above 200 °C. Peoples used the geothermal energy resources for bathing, cooking and heating. Hot water near the earth's surface can be piped directly into buildings and industries for heat. A district heating system provides heat for 95% of the buildings in Reykjavik, Iceland. Examples of other direct uses include: growing crops, and drying lumber, fruits, and vegetables.

Thermodynamic properties of the Guba region geothermal waters were analysed: the chemical compounds of samples were analysed in the IRIS Intrepid II Optical Emission Spectrometer (U.K.). The IRIS Intrepid II Optical Emission Spectrometer Series is a family of inductively coupled argon plasma (ICP) optical emission spectrometers (OES) which use Echelle optics and a unique Charge Injection Device (CID) solid-state detector to provide superb sensitivity and selectivity. These systems provide complete and continuous wavelength coverage over the analytical wavelength range from 165 to 1000 nm.

The new denisty measurements at T=(278.15 to 413.15) K, p=(0.101 to 100) MPa were carried out. The temperature in the measurement cell, where the U–tube is located, is controlled using a thermostat with a  $\Delta T = \pm 10 \text{ mK}$  uncertainty of the measurement and is measured using the (ITS-90) Pt100 thermometer with a  $\Delta T = \pm 15 \text{ mK}$  experimental uncertainty of the measurement. Pressure is measured by pressure transmitter P-10 with an APD in 0.1 % of the measured maximum value.

The vapor pressure measurements were carried out using the two high-accuracy static experimental set ups. The glass cells are used for vapor pressures lower than ambient pressure at temperatures T = (274.15 K to 323.15) K and the metal cell for vapor pressures at the temperatures T = (323.15 K to 413.15) K.

An empirical correlation for the density and vapour pressure of the geothermal water has been developed.

#### **KEYWORDS**

Geothermal resources, density, vapor pressure, viscosity, vibration tube densimeter, equation of state, isothermal compressibility, thermal expansibility.

## THERMODYNAMIC FUNCTIONS OF MELTING AND PHASE TRANSITIONS OF THE A<sub>8</sub>GeX<sub>6</sub> (A=Ag, Cu; X=S, Se) COMPOUNDS

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Argyrodite family compounds with the general formula  $A_8B^{IV}X_6$  (A-Cu, Ag;  $B^{IV}$ -Si, Ge, Sn; X-S, Se, Te) have mixed ion-electronic conductivity, which makes them very promising for use in the development of photoelectrode materials, electrochemical solar energy converters, ion-selective sensors, etc. [1-3]. Most compounds of this class have phase transitions at relatively low temperatures (40-250 °C) [1, 4, 5]. The thermodynamic functions of the phase transitions of these compounds have not been studied.

The aim of this work was to determine the thermodynamic functions of melting and polymorphic transitions of compounds  $Ag_8GeS_6$ ,  $Ag_8GeS_6$ ,  $Cu_8GeS_6$  and  $Cu_8GeS_6$  by differential scanning calorymetry (DSC). The studies were carried out on a Linseis DSC400 differential scanning calorimeter using the *Linseis TA V 2.3.1* software, and the processing of the results was carried out using the *Linseis TA Evaluation V 2.3.1* software.

For the studies, ternary compounds  $Ag_8GeS_6$ ,  $Ag_8GeS_6$ ,  $Cu_8GeS_6$  and  $Cu_8GeS_6$  were synthesized by direct fusion of stoichiometric amounts of the corresponding high purity (99.999%) elementary components under vacuum in a two-zone furnace. Further, the samples were annealed at 500 ° C (100 h) and then at a temperature below the temperature of transitions of phase transitions of compounds (10 h). The synthesized compounds were identified by differential thermal analysis and powder X-ray diffraction technique.

Temperatures and heats of melting and polymorphic transitions of the  $Ag_8GeS_6$ ,  $Ag_8GeS_6$ ,  $Cu_8GeS_6$  and  $Cu_8GeS_6$  compounds were determined from heating curves. Based the values of the molar enthalpies of phase transitions, their molar entropies were calculated. Analysis of the data obtained showed that the entropies of polymorphic transitions of the studied compounds have anomalously high values. This is probably due to the strong disordering of silver and copper cations upon transition to the high-temperature superionic cubic modification.

#### ACKNOWLEDGMENT

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## PHASE BEHAVIOR OF HYDROCARBON MIXTURES FOR THE LOW CONCENTRATION OF HEAVY COMPONENTS

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A method of precision adiabatic calorimetry for investigation of phase equilibria of hydrocarbon mixtures for the low concentration of heavy hydrocarbon components ( $C_{4+}$ ) was applied. The ternary and four-component hydrocarbon systems, methane + propane + octane, methane + propane + decane, methane + propane + octane + decane have been studied. Heat capacity, internal energy, pressure, and temperature derivative of pressure at constant volume for these systems have been measured in the range of 100–370 K and 0.1–40 MPa. Phase diagrams have been plotted based on the experimental data of heat capacity, internal energy, pressure, and temperature derivative of pressure at constant volume. Phase transitions are localized by the finite discontinuities in temperature derivatives of the thermodynamic potentials.

A quasi-binary approximation allows us to reveal an impact of heavy hydrocarbons to the phase behavior of a hydrocarbon mixture. A first quasi-component is a binary mixture with the constant methane/propane ratio. A second component is a component of the  $C_{4+}$  fraction. Variation of the concentration of a second component allows us to reveal its impact to the phase behavior of a mixture.

Our investigations show the phase behavior of a hydrocarbon mixture for the low concentration of heavy hydrocarbon components is drastically transformed compared to the customary concept.

- The hydrocarbon mixture splits into a macroscopic phase (a macrophase enriched by methane and propane) and microscopic phases (microphases enriched by heavy hydrocarbon components).
- Each microphase consists of one heavy hydrocarbon component.
- The phase behavior of each microphase in four-component system methane + propane + octane + decane doesn't depend on concentration of other heavy component.
- The high molecular components provoke the splitting of liquid part of a macrophase into two liquid phases.

To prove that all phases are equilibrium phases a cooling mode of measurements was used. At the cooling mode of measurements the same phase transitions as at the heating mode occurred. These phase transitions correspond to the formation of microphases enriched by the hydrocarbon heavy components and a macrophase enriched by methane and propane.

#### ACKNOWLEDGMENT

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# THERMODYNAMIC AND THERMOPHYSICAL PROPERTIES OF DRY AIR BY USING SCHREIBER-PITZER EoS FOR GAS MIXTURES

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Dry air is one of the most used gases in industrial and technological applications. In dry air thermodynamic property calculations, it is usually ideal gas EoS is used. The basic reason for this is the simplicity of using ideal gas EoS. For most applications, it might be sufficient, but when applications with higher pressure zones are considered, error level will increase. An equation of state with better accuracy of thermodynamic properties will be required for extreme cases and Schereiber-Pitzer equation of states (EoS) for dry air is considered in this paper. So, the objective of this study is to supply to researchers a more accurate EoS for dry air compare to ideal gas EoS for thermodynamic and heat transfer analysis. Set of computer programs were developed in java language in order to calculate thermodynamic properties like specific volume, internal energy, enthalpy, entropy, Gibbs energy, Helmholtz energy, specific heat and thermophysical properties such as thermal conductivity and viscosity of dry air. The results are compared with perfect gas EoS, Peng-Robinson EoS and EoS developed by The International Association for the Properties of Water and Steam (IAPWS).

**Keywords:** Thermodynamic properties of dry air, thermophysical properties of dry air, Peng-Robison EoS, cubic EoS.

# KINETIC AND THERMODYNAMIC STUDY OF THE ANTICANCER ACTIVITY OF FULLERENE NANOSTRUCTURE DERIVATIVES. EXAMPLE OF THE ELIMINATION OF THE CARCINOGENIC AGENT BENZO ALPHA PYRENE (BaP) FROM BIOLOGICAL SYSTEMS. DFT CALCULATION

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In this work, the reaction of fullerenes with a carcinogenic agent, BaP will be studied in order to eliminate BaP from biological systems. The thermodynamic and kinetic calculations will be carried out with the aim of showing that by functionalizing C60 with groups such as OH, CH<sub>2</sub>OH, CONH<sub>2</sub> and COOH, the band gap will decrease and the aromaticity and the polarity of the cycles will increase, therefore, with more reactivity and solubility of the functionalized C60, we will examine the cycloaddition [2 + 2] reaction of BaP with the C<sub>60</sub> initiations. Using the DFT methods we will show that C<sub>60</sub>CONH<sub>2</sub> with a higher dipole moment, a higher electrophilicity, a lower reaction energy, an enthalpy and an enthalpy free minimized and also due to the creation of additional bonds between CONH<sub>2</sub> and BaP in the structure C<sub>60</sub>-CONH<sub>2</sub> 2.5 BaP, is inspired as a favorable compound for biological anticancer activity.

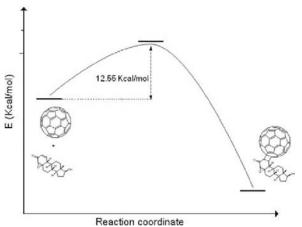


Figure 1. Fullerene and BaP [2+2] cycloaddition mechanism.

**KEYWORDS:** nanotechnology, fullerenes, anticancer activity, kinetic and thermodynamic prosperities, DFT calculations.

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# STUDY OF ANTIMICROBIAL PROPERTIES OF CYCLOHEXANONE COMPOUNDS

#### Narmina GULIYEVA, Zahida ALIYEVA, <u>Murad MALIKZADE</u>, Nubar MALIKOVA, Ramin ABDULLAYEV, Madina ALIYEVA, Qasham HAJIYEV

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1,3-Dicarboxylates and cyclohexanols are two of the main directions of organic synthesis. Because of 1,3-dioxo fragments that are contained in the structure of the mentioned type compounds, it becomes possible to proceed annelated bicyclic systems mainly containing five-membered heterocycles. Heterocyclic substances such as 1,3-Dicarboxylates and cyclohexanols can be used as inhibitors of cancer cells. Heterocycles contain heteroatoms and can change their antimicrobial properties. That means Sulfur, Nitrogen, Oxygen and spirocycles (according to their structures) change the antimicrobial properties of the heterocycle. New heterocycles that we synthesized have various properties. Thus, the primary heterocycle contains a Nitrogen-containing spirocycle. On the other hand, the second heterocycle contains Nitrogen and Sulfur, but its structure is not spirocycle. In conclusion, experimental results suggest that spirocycle-based heterocycles have better antimicrobial properties than sulfur-based heterocycles.

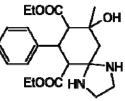


Figure 1: (diethyl-9-hydroxy-9-methyl-7-phenyl-1,4-diazaspiro [4.5] decane-6,8dikarboksilat)

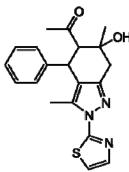


Figure 2: (1-(-6-hydroxy-3,6-dimethyl-4-phenyl-2-(thiazol-2-yl)-4,5,6,7-tetrahydro-2H-indazol-5-yl) ethan-1-one).

# HYDROCRACKING OF VACUUM GASOIL

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The future of oil refining industry directly depends on its adaptation to new market structures of oil refineries. The main objective of oil refining industry in the last decade is producing environmentally-friendly gasoil and diesel fuels. The problems of increasing oil refining depth and obtaining commercial products meeting the modern requirements may be solved by the development of new methods for refining the fractions obtained by the re-refining processes, as catalytic cracking, hydrocracking, viscracking, coking.

Recently, economic and environmental problems cause a rapid growth in diesel engines. It's necessary to meet demands of national economy for diesel fuel in connection with the use of it in many countries. Hydrocracking process is the most efficient one of re-refining processes for obtaining diesel fraction from a heavy petroleum raw material. Hydrocracking isn't only additional resource for obtaining diesel fraction, simultaneously one of the efficient methods for hydroenrichment of catalytic cracking raw material.

The correct selection of catalysts is the main factor for successful realization of different raw materials hydrocracking in industry. Simultaneously with high hydrodesulfurization activity, these catalysts should have high hydrogenation and decomposition abilities at low temperatures for a complete hydrogenation of unsaturated, diene and partially polycyclic aromatic hydrocarbons. These hydrocarbons causes not only reduction in thermal stabilities of fuels, but also a rapid coking of technical equipments in the further refining [1].

Oxides or sulfides of the VI and VIII elements of the periodic table are used individually or as different compounds to realize hydrogenation function. Efficient hydrocracking catalysts contain molybdenum, nickel, cobalt, tungsten, precious metals – platinum, palladium and etc. The most common acid carriers are amorphous and crystalline inorganic oxides: aluminum oxide, amorphous aluminum silicates and magnesium silicates, crystalline aluminum silicates [2].

Recently, the researches have been carried out at IPCP of ANAS in the direction of heavy petroleum residues (fuel oil, tar) hydrocracking. Currently, for the purpose of carrying out vacuum gasoilhydrocracking process the researches are being carried out in the direction of the synthesis of domestic aluminosilicate catalyst with transition metals and hydrocracking of the vacuum gasoilobtained from Azerbaijani petroleums for the purpose of obtaining low sulphurous raw material for high-quality diesel fuel and catalytic cracking process in the presence of this catalyst. The tests were carried out at 400-450°C, under 3-8 MPa, 0.6-2 h<sup>-1</sup> volume velocity. According to preliminary results, it's possible obtaining low sulphurous raw material for catalytic cracking process, simultaneously with environmentally-friendly diesel fuel.

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# THERMOPHYSICAL PROPERTIES OF IONIC LIQUIDS WITH [TFO] ANIONS

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lonic liquids (ILs) are liquid salts at the ambient temperatures. They are ideal solvents for green chemistry, have negligible vapor pressure, non-flammable, low melting point, high solvating capacity, low compressibility, high ionic conductivity, high thermal, mechanical and electrochemical stability etc., which make them attractive for practical applications. Due to these unique characteristics make ILs suitable in the various branches, for example as media for the separation of gases from mixtures, as CO<sub>2</sub> removal from flue-gas streams by absorption, as thermal storage media and heat transfer fluids. In order for design and developing reliable predictive models and to understand the nature of molecular interactions in liquid mixtures and to decide whether the IIs are suitable as a part of novel working pair, the basic thermodynamic properties (density, viscosity, heat capacity, compressibility, thermal expansion coefficient etc.) are required.

This work is a continuation of our investigations in the field of  $(p,\rho,T)$  properties of ILs. The new accuracy  $(p,\rho,T)$  data of 1-alkyl(C<sub>2</sub>, C<sub>4</sub>, C<sub>6</sub>, C<sub>8</sub>)-3-methylimidazolium trifluoromethanesulfonate [C<sub>n</sub>MIM]<sup>+</sup> [TFO]<sup>-</sup>, where n = 2, 4, 6, 8, ILs at the wide T = (273.15 to 413.15) K range of temperature and pressures up to p = 140 MPa are reported. The temperature in the measuring cell was measured with an expanded absolute uncertainty of U(T) = 0.015 K. Pressure was measured using a pressure transmitters P-10, P-30 (0.25, 2.5, 50, 100 MPa) and HP-1 (160 MPa) with an expanded relative standard uncertainties U of  $(p,\rho,T)$  measurements in: U(p) = 0.00025 MPa for p < 0.25 MPa, U(p) = 0.01 MPa for p < 100 MPa, U(p) = 0.25 MPa for p < 100 MPa. According to the specifications of Anton Paar and calibration procedures performed in our laboratory, the observed repeatability of the density measurements at all T = (263.15 to 468.70) K temperature range of DMA HPM vibration tube densimeter and pressures up to p = 140 MPa, also attending the high viscosity corrections to vibration tube periods have an expanded uncertainty within  $\Delta p/\rho = \pm (0.01 \text{ to } 0.08)\%$ .

The ambient pressure density  $\rho(p_0, T)$  values were measured using Anton Paar DMA 5000M, DSA 5000M and DMA HPM vibrating tube densimeters with an uncertainty in  $\Delta \rho = \pm (5 \cdot 10^{-3} \text{ to } 3 \cdot 10^{-1}) \text{ kg} \cdot \text{m}^{-3}$ . The heat capacities  $c_p(p_0, T)$  of ILs at ambient pressure and various temperatures were measured using the DSC Pyris 1 calorimeter.

An empiric equation of state for fitting of the  $(p,\rho,T)$  data has been developed as a function of pressure, temperature and molecular mass of  $[C_nMIM]^+$  [TFO]<sup>-</sup> ILs. This equation together with the heat capacity values was used for the calculation of the thermophysical properties of these ILs, such as isothermal compressibility  $\kappa_T(p,T)/MPa^{-1}$ , isobaric thermal expansibility  $\alpha_p(p,T)/K^{-1}$ , thermal pressure coefficient  $\gamma(p,T)$  /MPa·K<sup>-1</sup>, internal pressure  $p_{int}(p,T)/MPa$ , specific heat capacities  $c_p(p,T)/J\cdot$ kg<sup>-1</sup>·K<sup>-1</sup> and  $c_v(p,T)/J\cdot$ kg<sup>-1</sup>·K<sup>-1</sup>, speed of sound  $u(p,T)/m\cdots^{-1}$ , isentropic expansibilities  $\kappa_s(p,T)$  at high pressures and temperatures, in which the density of [C<sub>n</sub>MIM]<sup>+</sup> [TFO]<sup>-</sup> ILs were measured. The available literature values of these ILs were compared with obtained in this work values

# COMPARATIVE STUDY OF SCALE INHIBITION ABILITY OF SCHIFF BASE AND CORRESPONDING CROWN-ETHER

#### Sarvinaz HAJIYEVA<sup>1</sup>, Konul AMRALIYEVA<sup>2</sup>, Ulviyya HASANOVA<sup>1</sup>, Mirjavid AGHAYEV<sup>1</sup>

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Salt deposition has an extremely negative impact on pipeline safety. It can cause local corrosion of pipes metal, which leads to their rapid destruction and creates a fire hazard in the pipelines. The number of failures in oil and gas industry is due to the development of local corrosion in pipelines and is a big part of total accidents. The situation is aggravated by the fact that it is very difficult in practice to identify local corrosion areas of pipelines. The salt layer increases energy consumption during oil transportation and this leads to significant economic losses [1]. Salt deposition occurs during all well operation methods, but the most negative consequences of salt deposition are observed when oil production is carried out by electric submersible pumps (ESP). These types of pumps are highly sensitive to calcium carbonate scales, because high pressure and temperature sufficiently contributes to the deposition of CaCO<sub>3</sub>[2].

Analysis of salt deposits in Caspian basin shows that most of them belong to the calcite type. Considering the fact that application of ESP with high probability of scale formation requires chemical treatment, we decided to investigate in this study the salt formation inhibitors based on Schiff base and crown-ether with similar structure. The presence of hydrophilic amine groups in organic inhibitor (electron donating functional group) is important due to their high adsorption on the metal surface and the formation of the Langmuir–Blodgett film, in which the hydrophobic alkyl part of the molecule pushes water molecules over the metal. Schiff bases and their reduced derivatives are showing good inhibitor activity, also their activity highly depends on the presence and ratio of hydrophobic and hydrophilic groups [3, 4]. Crown ethers, in their turn, are efficient and selective chelators for different cations and can also contain nitrogen, oxygen and sulphur atoms in their cavity, which also facilitates their binding to the metal surface.

In present study was synthesized and investigated the structure of Schiff base on the basis of L-lysine and salicylic aldehyde (2,6-bis-(2-hydroxybenzylidene)amino)hexanoic acid. For the first time was synthesized its macroheterocyclic derivative (8,9,10,11,19,20–hexahydro-7H-dibenzo[1,4,8,14] dioxadiazacycloheptadecine-7-carboxylic acid) by the consequent substitution reaction with 1,2-dibromoethane. The inhibitor activity of both compounds was investigated, in order to determine whether the cyclization process affects it.

The methods applied in this study are <sup>1</sup>H, <sup>13</sup>C NMR, UV-Vis and FTIR-spectroscopy and SEM, EDS of treated and untreated steel surface.

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# REFINEMENT OF THE PHASE DIAGRAM OF THE BI-Te SYSTEM AND THERMODYNAMIC PROPERTIES OF BISMUTH TELLURIDES

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Bismuth tellurides with a tetradymite-like layered structure are of great interest as polyfunctional materials that combine the topological insulators properties with thermoelectric, optical, magnetic etc. ones [1-5]. However, the known phase diagram of the Bi-Te system does not reflect all compounds formed in the system. This paper presents the results of refinement of the phase diagram of this system and the thermodynamic properties of bismuth tellurides.

The alloys were synthesed by the fusing stoichiometric amounts of elementary components in evacuated quartz ampoules at 650°C with subsequent quenching in cold water. Then, alloys were annealed at 250 °C (<30 at% Te), 350 °C (30-45 at% Te) and 400 °C (> 40 at% Te) for 800-1000 h. The studies were carried out by DTA (NETZSCH 404 F1 Pegasus differential scanning calorimeter), XRF (Bruker D8 ADVANCE powder diffractometer) and measurement of the EMF of concentration cells of the type

in the 27-170 °C temperature range. The electrochemical cell assembly and measurements are described in detail in [6].

Based on the experimental data, it was established that in the system, in addition to  $Bi_2Te_3$  with congruent melting at 587 °C, the following compounds are formed that melt incongruently according to peritectic reactions:  $Bi_4Te_5$  (562°C),  $Bi_8Te_9$  (550°C), BiTe (539°C),  $Bi_4Te_3$  (435°C),  $Bi_2Te$  (392°C),  $Bi_7Te_3$  (330°C). The types and parameters of the crystal lattices of these compounds were determined from the data of powder diffraction patterns.

Linear equations of the E = a + bT type for various phase regions of the system were obtained from the measurements of (1) type cells, from which the partial thermodynamic functions of bismuth in alloys were calculated. Based of the phase diagram, potential-forming reactions for the above bismuth tellurides were determined and their standard Gibbs energies of formation and enthalpies of formation, as well as standard entropies, were calculated. The values obtained for  $Bi_2Te_3$  are in good agreement with the literature data, and for other compounds were determined for the first time

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# SYNTHESIS OF STABILIZATION OF NICKEL NANOPARTICLES WITH POLYACRYLIC ACID

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Nanomaterials have been carefully studied from fundamental scientific and technological interest to enter new classes of functional materials with different properties and applications. In recent years, nickel nanoparticles have been used in chemical catalysis, electrocatalysis, dyes, magnetic notes, rechargeable batteries, medical diagnostics, superconducting devices and so on are applied from different perspectives in the fields. Among the various synthetic approaches developed, the chemical solution phase can be provided in a variety of ways to gain control over particle size, morphology, crystal phase, and other suitable relationships.

According to our experiments, polymers can stabilize metal nanoparticles through the steric mass of their frames and also bind weakly to the nanoparticle surface by heteroatoms acting as ligands. It has been also reported that polymers can control the shape and size of nanoparticles. Also, polymer-stabilized metal nanoparticles can be dispersed uniformly in organic solvents or water and mixed with reagents and products in a manner similar to homogeneous catalytic systems, using polyacrylic acid and organized as a stabilizer. The reduction of nickel chloride in aqueous solution with sodium borohydride results in electrochemically active nickel nanoparticles with sufficient monodisperse and separate use of a single-coated polymer such as polyacrylic acid (PAA). The size of Ni nanoparticles is very small and can be easily adjusted by changing the polymer and concentration in each situation. At selected concentrations of polymers that provide a similar number of monomer units, polyacrylic acid performs very well as a stabilizer. Research shows that polyacrylate anions with high positive potential interact more with catalyst nanoparticles. Different pH = 4... 9 was created to study the effect of acidic environment on the dispersion of suspensions of nickel nanoparticles. The pH was equalized with 1% HNO<sub>3</sub> and NaOH using acid-based titration.

### THE USE OF IRON NANOPARTICLES FOR WATER PURIFICATION

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Given that iron has different oxidation states and is widespread in nature since it is non-toxic and environmentally friendly, we have done the work and prepared a membrane component based on synthesized iron nanoparticles on carriers of different structures for water purification. We synthesized iron nanoparticles with zero valency.

In virtue of size, nanomaterials have been shown to acquire distinguishing chemical, electronic, optical, mechanical, magnetic, and catalytic properties. Over the last 27 years, as a result of the multidisciplinary nano 'boom' in the mid-1990s, various methods have been developed for the synthesis of nanoscale particles and these particles have been applied increasingly for a vast amount of applications: from drug delivery to novel methods of treatment of environmental remediation and hazardous waste treatment.

Taking into consideration that iron in different oxidation states is widely distributed in nature, so it is non-toxic and biofriendly towards the environment we prepared the membrane component on the basis of synthesized supported iron zero-valent nanoparticles for purification of water contaminated with nitrate and dichromate ions. We are interested particularly in supported nanoscale zero-valent iron (nZVI) due to its mild reducing properties and biocompatibility that can be used in green environmental technologies. Reactions of ZVI with some contaminants including Cr(VI) (1) and nitrates (2) are given as follows:

$$2CrO^{4-}+3Fe^{0}+10H^{+}\leftrightarrow 2Cr(OH)_{3}+3Fe^{2+}+2H_{2}O$$
(1)  

$$4Fe^{0}+NO^{3-}+10H^{+}\rightarrow 4Fe^{2+}+NH_{4}^{+}+3H_{2}O$$
(2)

A crucial challenge of nZVI used in environmental applications is its strong propensity of agglomeration, prompt sedimentation and accordingly limited mobility in the aqueous environment. The main approach for improving zero-valent iron nanoparticles stability is using appropriate stabilizer.

Therefore our principal objective is aimed not only on the synthesis of ZVI nanoparticles but also on stabilization and its possible application in membrane technology for remediation of contaminated water.

We synthesized ZVI nanoparticles based on potassium borohydride reduction method of iron sulfate heptahydrate. The reduction of Fe<sup>2+</sup> to Fe<sup>0</sup> occurs corresponding to the following reaction:

Fe <sup>+2</sup> + BH <sup>4-</sup> + 6H<sub>2</sub>O → Fe <sup>0</sup> + 2B(OH)<sub>3</sub> + 7H<sub>2</sub> 
$$\uparrow$$
 (3)

We identified the most promising pathway of synthesis in order to obtain iron nanoparticles with the best stability and mobility, by comparing the above given techniques. Have been found out that the coating of ZVI nanoparticles by stabilizers after carrying out of actual reduction reaction leads to a more homogenous distribution of prepared ZVI NPs in terms of their size and morphology.

# STUDY OF THE PROCESS OF OLIGOMERIZATION OF C6-C8 $\alpha$ -OLEFINS IN THE PRESENCE OF A NEW CATALYTIC COMPLEX BASED ON ALUMINUM MODIFIED CuCl<sub>2</sub>

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Currently, aluminum compounds in the catalysis space are considered as perspective materials. After removing of the passive oxide layer, aluminum is easily reacted with proton-donor and halogen compounds. The active aluminum chloride catalytic complex (CTC/Cu) was synthesized in situ mode with its 1.2-dichloroethane and CuCl<sub>2</sub> interaction, using the activated form of aluminum. The usage of the synthesized catalytic complexes in transformations of olefins makes it possible to give up massive or saturated AICI<sub>3</sub>, which is a series of deficiencies (catalyst activation, difficulty in controlling the reaction, its high consumption, hygroscopicity, etc.). In this regard, the synthesis of CTC/Cu was carried out at a temperature of 80-85°C for 20-22 hours. The structure and properties of the catalytic complex were studied, and olefins were oligomerized in its presence and extensive studies were conducted on the physical and chemical properties of the oils received. It has been established that the paraffin hydrocarbons which were used as solvent in the process play an important role as H-donor to the formation of the catalytic complex. The composition and properties of CTC/Cu were investigated by using EMR, TQ, DTQ, UV, IQ-spectroscopy, RFA, RFM methods. It has been established that during the synthesis of CTC/Cu, along with the active catalytic centers containing aluminum chloride, nanocarbon particles are also formed that form paramagnetic properties in the form of clusters of 30-200 nm which are interact with each other. On the basis of carried out researches, it is possible to tell that delocalized electronic particles Cn are formed in an alumochloride complex interacting with catalytic centers, at the expense of formation of clusters in the process of oligomerization CTC/Cu shows high stability in comparison with CTC and catalysts which contain AICl<sub>3</sub>. The synthesized CTC/Cu were used in the individual and joint oligomerization process of C<sub>6</sub> and C<sub>8</sub> a olefins and the effect of temperature, reaction time, density of catalyst in the process was investigated. It has been established that the degree of oligomerization of olefins depends directly on the density and temperature of the catalyst. The CTC/Cu with 0.5% concentration behaves markedly active at temperature of about 60°C, that promotes the increasing output of oligomerization product to 92-94% concentration over 2h. In the given optimal conditions, it is possible to obtain oligomers characterized by narrow molecular mass distribution with having high output and viscosity index (110-132) during oligomerization of  $C_6$  and  $C_8 \alpha$ -olefins with the presence of CTC/Cu (Tab.1).

	Olefins		
Parameters	Hexene-1 (C <sub>6</sub> )	Octene-1 (C <sub>8</sub> )	C <sub>6</sub> and C <sub>8</sub> mixture 1:1 (mol)
Density g/sm <sup>3</sup>	0,8334	0,8366	0,8437
Kinematic viscosity, mm <sup>2</sup> /s, (40°C)	21,466	29,548	25,215
Kinematic viscosity, mm <sup>2</sup> /s, (100°C)	4,3172	5,6190	6,9832
Viscosity index	110,4	129,7	132,7
Refractive index	1,4625	1,4692	1,4719

Table 1. Obtained results of oil fractions at T> 400°C in the presence of CTC/Cu

# OBTAINING OF NANOSTRUCTURED γ-Al<sub>2</sub>O<sub>3</sub> BY SOL-GEL METHOD

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The Sol-gel method is indispensable in the efficient phase condensation of nanoparticles. Advantages of this method are low temperature, high homogeneity and monodispersity, ability to control nanoparticle's sizes, synthesis of multicomponent systems and, most importantly, easy implementation in laboratory conditions. It should also be noted that the nanoparticles which obtained within the sol-gel method are aggregative sustainable. In recent years, intensive research has been carried out to obtain metal nanoparticles by using the sol-gel method. These studies involve the production of hydroxide from various salts in the presence of stabilizers, acquisition of metal oxides or metal nanoparticles within pyrolysis by CVD in an inert environment and the study of physical properties by various methods.

In the present work, has been investigated synthesis of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> by the sol-gel method and by using this as a catalyst in the process of obtaining nanocarbon from pyrolysis of natural gas. In the process, monoethanolamide (MEA) was used as a precipitator and stabilizer, it has been established that the MEA provides the formation of high-dispersion (5-20 nm) particles. The synthesis within the sol-gel method was investigated in the MEA/AI = 1.0-3.0 range, and the optimal condition was chosen for the process.

Initially, the aluminum nitrate solution was hydrolyzed with the presence of monoethanolamide at a temperature of 40 °C by formulation of sol, then the monolithic gel is formed as a consequence of the formation of more durable bonds by raising the temperature of the disperse phase to 90 °C. The gel was dried at 200 °C in the CVD reactor for 2 hours, afterwards nano  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> was dehydrated at 850 °C and analyzed within various physical methods.

X-ray diffraction was used for determine the dependence between the obtained gel structure and the phase composition. It was found that the amorphous structure is retained to 400 °C, the cubic crystal cage samples begin to form after 400 °C, and at 850 °C small crystalline structure with a diffraction maximums are noticeable. The results of XP analysis prove that the synthesized sample consists mainly of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> phase.

The morphological characteristics of the sample was investigated and determined by electron microscopy. Synthesized particles of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> have fibrous structure and have dimensions in nanometer range.

# SOLID SOLUTIONS BASED ON Cu<sub>3</sub>SbSe<sub>4</sub> IN THE Cu<sub>3</sub>SbSe<sub>4</sub>-SnSe<sub>2</sub> (GeSe<sub>2</sub>) SYSTEMS

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Ternary chalcogenides of copper and silver for many years have attracted the attention of researchers due to the fact that many of them exhibit photoelectric, thermoelectric, optical, and other properties, as well as mixed electron-ionic conductivity [1-3]. In particular, synthetic analogs of copper minerals: tetraedrit Cu<sub>12</sub>Sb<sub>4</sub>S<sub>13</sub>, chalcostibite (CuSbS<sub>2</sub>(Se<sub>2</sub>)), permingeatite (Cu<sub>3</sub>SbSe<sub>4</sub>), skinnerite (Cu<sub>3</sub>SbS<sub>3</sub>) etc. are of great practical interest due to the possibility of developing new environmentally friendly thermoelectric materials on their basis [4-7]. One of the ways to optimize the functional properties of known compounds is to obtain solid solutions on their basis.

This work is a continuation of our research on the search for complex phases of variable composition based on copper chalcogenides [8-10] and devoted to study the solubility based on the Cu<sub>3</sub>SbSe<sub>4</sub> compound in the Cu<sub>3</sub>SbSe<sub>4</sub>-GeSe<sub>2</sub> (A) and Cu<sub>3</sub>SbSe<sub>4</sub>-SnSe<sub>2</sub> (B) systems. The initial compounds of the studied systems were synthesized by fusing high-purity (99.999%) elementary components in the required ratios in evacuated up to ~10<sup>-2</sup> Pa and sealed quartz ampoules at temperatures 50 °C higher than their melting temperatures in a two-zone furnace. The alloys of the studied systems, each weighing 0.5 g, were obtained by fusing stoichiometric amounts of the previously synthesized and identified starting compounds under vacuum at 700 °C with further annealing at 400 °C for 500 h. The alloys were studied by means of differential thermal analysis, powder X-ray diffraction technique and scanning electron microscopy.

A joint analysis of the experimental results showed that the solubility based on the Cu<sub>3</sub>SbSe<sub>4</sub> compound in system (A) is at least 15 mol% GeSe<sub>2</sub>, and in system (B) at least 20 mol% SnSe<sub>2</sub>. In alloys with compositions outside the homogeneity regions, a complex picture of phase equilibria in both studied systems is observed, leading to their instability below the solidus.

Thus, in spite of the different crystal structures of the initial compounds in the studied systems, rather wide ranges of solid solutions based on  $Cu_3SbSe_4$  are formed. Apparently, this is due to the fact that, when the antimony ions  $Sb^{5+}$  are replaced by  $Ge^{4+}$  ( $Sn^{4+}$ ) ions, the difference in their charges is compensated due to the transition of some of the  $Cu^+$  ions to the  $Cu^{2+}$  state.

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# AN OPTICAL METHOD FOR STUDYING PHASE BEHAVIOR OF THE NEAR-CRITICAL HYDROCARBON FLUIDS

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An efficient optical method is proposed for identifying and studying the near-critical state of formation hydrocarbon (HC) fluids located in the transition zone from volatile oil to gas condensate, i.e. at reservoir temperature close to critical. The development of deposits of such fluids requires reliable knowledge of not only critical parameters, but also the area of their near-critical state.

The method uses the well-known phenomenon of critical opalescence - an anomalous (ideally, unlimited for forward scattering) increase in the intensity of light scattering with approaching the critical point liquid-gas. The essence of the method consists in measuring the temperature dependence of the intensity of light scattering by the studied fluid on a sequence of isochores covering the region of critical opalescence, and fixing the temperatures of the maxima of sharp lambda-shaped peaks in the intensity of light scattering associated with the transition of the fluid to a two-phase state. The region of the observed critical opalescence is taken as the region of the near-critical state of the HC fluid. In turn, the position of the boundary dew-bubble curve of the fluid in the near-critical region is determined by the maxima of the sharp lambda-shaped peaks of the measured intensity of light scattering on the passed isochores. In turn, the position of the boundary dew-bubble curve of the fluid in the near-critical region is determined by the maxima of the sharp lambda-shaped peaks of the measured intensity of light scattering on the passed isochores. Finally, the position of the critical point of the fluid under study on the experimentally determined boundary curve is determined from the absolute maximum (maximum of the maxima) of the measured light scattering intensity among all the passed isochores.

In the field of the availability of optical measurements, the method solves the problem of reliable determination of the critical parameters of thermally stable HC fluids and claims to become a standard for studying their nearcritical phase behavior. This method can be easily integrated into standard PVT installations and can serve as the basis for the criterion for determining the transient (near-critical) class of formation fluids.

Approbation of the method on a number of model and reservoir HC mixtures has shown its high practical otential. In particular, for the first time on the phase diagram of a real reservoir HC mixture in temperature – pressure variables, in addition to the boundary dew-bubble curve and the position of the critical point, the region of the nearcritical state is shown, characterized by anomalies of a number of basic thermodynamic quantities.

#### ACKNOWLEDGEMENTS

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Available from: http://vesti-gas.ru/sites/default/files/attachments/vgn-5-37-2018-201-211.pdf

# **ISOBAR HEAT CAPACITY OF GASEOUS AND SUPERCRITICAL HYDROCARBONS**

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A criterion for the thermodynamic similarity of the properties of hydrocarbons in the gaseous and supercritical states in the regions of their sharp change is proposed, taking into account the structure of their molecules and the potentials of intermolecular interaction. The critical temperature  $T_c$  and the isobaric heat capacity in the state of an ideal gas at  $T = 0.74T_c$  are taken as individual constants of hydrocarbons that determine their behavior in the indicated regions of state parameters. This temperature corresponds to the absolute minimum of the free energy of the liquid-vapor phase transition process. Then:

$$K = \left(\frac{C_p^0}{C_{p(et)}^0}\right)_{T=0,74T_c}$$
$$C_p(\pi,\tau) = C_{p(et)}(\pi,\tau) * K$$

where  $C_{p(et)}$  is the isobaric heat capacity of the "reference" hydrocarbon,  $\pi = P/P_c$  and  $\tau = T/T_c$ .

A comparative method for calculating the heat capacity of gaseous hydrocarbons of the methane series at reservoir temperatures and pressures ( $0.6 < \tau \le 1.2$  and  $0.03 < \pi < 0.92$ ) and a program for its numerical implementation by the method of constructing a neural network have been developed (State certificate of the Russian Federation on registration of computer programs No. 2011618328).

A comparative method for calculating the heat capacity of hydrocarbons in the supercritical region of maximum heat capacity at 0.7 < $\tau \le 1.2$  and 1.05 < $\pi < 2$  and a program for its numerical implementation by the interpolation method using the variable degree Lagrange polynomial have been developed (State certificate of the Russian Federation on registration of computer programs No. 2012612289).

Normal heptane was taken as the "reference hydrocarbon", since it was experimentally investigated in sufficient detail and reliably in the indicated interval of  $\tau$  and  $\pi$  by the method of a flow-through adiabatic calorimeter with calorimetric flow measurement [1]. Comparison with the most reliable literature data on the isobaric heat capacity of the experimentally investigated hydrocarbons showed their agreement, comparable with those calculated by the equations of state in the indicated ranges of state parameters.

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**KEYWORDS:** isobaric heat capacity, thermodynamic similarity, hydrocarbons, calorimeter

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# SOLID-PHASE EQUILIBRIUM DIAGRAM OF FeSe-Ga<sub>2</sub>Se<sub>3</sub>-In<sub>2</sub>Se<sub>3</sub> SYSTEM

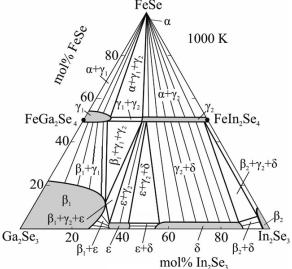
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Magnetic semiconductors of the AB<sub>2</sub>X<sub>4</sub> type (A - Mn, Fe, Co, Ni; B - Ga, In; X - S, Se, Te) and solid solutions based on them have unique physical properties, making them promising materials for use in the lasers, light modulators, photodetectors and other functional devices controlled by a magnetic field [1-3]. Development of new multicomponent phases and materials is based on data on phase equilibria in corresponding systems [4,5].

This paper presents the results of studying phase equilibria in the FeSe-Ga<sub>2</sub>Se<sub>3</sub>-In<sub>2</sub>Se<sub>3</sub> system by DTA (NETZSCH 404 F1 Pegasus system, platinum-platinum-rhodium thermocouples) and XRD (D8 ADVANCE diffractometer from Bruker, CuK<sub>a</sub> radiation). To study this system, the initial binary compounds, as well as FeGa<sub>2</sub>Se<sub>4</sub> and FeIn<sub>2</sub>Se<sub>4</sub>, were first synthesized. The synthesis was carried out by direct melting of the high purity elementary components in evacuated (~10<sup>-2</sup> Pa) quartz ampoules in a two-zone furnace. The alloys of the system were prepared by the melting of the above-state compounds also under vacuum. To reach an equilibrium state, the ascast samples were subjected to thermal annealing at 1000 K FeSe for 500 h and then guenched in cold water.

Based on the experimental data, a solid-phase equilibria diagram at 1000 K was constructed (Fig.). It has been established that the system is characterized by the formation of limited regions of solid solutions based on the initial binary compounds ( $\alpha$ -,  $\beta_1$ - and  $\beta_2$ -phases). Also, intermediate  $\gamma_1$ and  $\gamma_2$ - phases were revealed along the FeGa<sub>2</sub>Se<sub>4</sub>-FeIn<sub>2</sub>Se<sub>4</sub> section and the  $\delta$ - and  $\epsilon$ -phases along the Ga<sub>2</sub>Se<sub>3</sub>-In<sub>2</sub>Se<sub>3</sub> boundary system. The indicated phases of variable composition form a number of two- and three-phase regions between themselves.



#### ACKNOWLEDGMENT

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# STUDYING THE STRUCTURE OF OLIGOMERIZATION PRODUCTS OF PROPYLENE OXIDE AND IMIDAZOLINES BASED ON DISTILLED NATURAL OIL ACIDS BY IR SPECTROSCOPY

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Progress in the oil industry, state export of oil and oil products are considered to be one of the inseparable parts of the global economic growth. However, along with the positive sites of economic integration, some disadvantages should be noted, particularly emergency situations happening during the transportation of oil and oil products. Accidents are unavoidable in oil production or transportation by water, which considers the elimination of the emergency spills consequences as necessary task requiring an immediate resolution. Accidents result in the loss of a huge amount of oil resources, and cause direct environmental threat to the fauna and flora of the hydrosphere. Surfactants are used to simplify the collection of a thin layer of oil after mechanical methods of cleaning the water surface. There are surfactants of various compositions, including products of oxypropylation of nitrogencontaining compounds which are known to be of great importance. In order to obtain new series of similar compounds, studies were carried out on the synthesis of oligomeric derivatives of imidazolines based on distilled natural petroleum acids and polyethylene polyamines with propylene oxide.

The synthesis process was implemented in an autoclave at a molar ratio of imidazoline to propylene oxide of 1: 5-15. The reaction was carried out with a moderate increase of temperature to the required value (~ 200 °C), which was determined by the onset of pressure reduction and continued until the pressure almost completely dropped. We revealed the complete conversion (~ 100%) of propylene oxide. The final product is a dark brown viscous liquid.

The structure of the synthesized oligomeric products was studied by IR spectroscopy. The following absorption bands were found on the IR spectra: deformation (1374, 1453 cm<sup>-1</sup>) and valence (2867, 2925, 2955 cm<sup>-1</sup>) vibrations of the CH bond of the CH<sub>3</sub> and CH<sub>2</sub> groups; valence (1644 cm<sup>-1</sup>) C = N bond vibrations; deformation (1546 cm<sup>-1</sup>) N – H bond vibrations (weak band); valence (3393 cm<sup>-1</sup>) vibrations of H-O bond of alcohol; valence (1011, 1087 cm<sup>-1</sup>) vibrations of the CO bond of alcohol.

It should be noted that the absorption band at 1731 cm<sup>-1</sup>, characteristic of the C = O bond, is observed on the spectra. Its presence can be explained by the possible isomerization of the formed alcohol fragments into aldehyde at high temperature. Similar peaks appear with low intensity.

Thus, all existing absorption bands, as well as the absence of bands characteristic of the epoxy cycle confirm the validity of the proposed reaction with the possible opening of the cycle between N-H fragments and alcohol groups resulting from the opening. Surveys are being conducted to study the properties and suitability of these oligomers as oil collecting and oil dispersing reagents.

# **ABSHERON OIL FIELD**

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Azerbaijan is an ancient oil and gas country. Absheron oil and gas district is the most perspective for oil reserves and oil production from eight oil and gas regions of our country. In accordance with the contract of the 20th century on the basis of Azeri, Chirag and Gunashli fields, which are included in this oil and gas region, bed oil is exported to foreign markets. The gas produced from the Shah Deniz field, which has a very rich gas reserves in that oil-gas region, will be exported to the world market via the TAP and TANAP lines under the 21st century agreement. The Absheron Cube oil field belongs to the sea oil of this region. Absheron oil fields is located in the northeast of Pirallahi. Investigation of Azerbaijan's need for efficient use of each oil field is crucial. As the Absheron Cube field oil is not yet explored, its composition and properties are considered to be actual issues. For this purpose, the physical and chemical properties of this oil have been determined. It has been established that the bed of Absheron cube was found to be low-toxic (0.31%), lowparaffin (1.09%) and high-grade (15.12%).. The Absheron field oil is distributed to 500° to 10°C by fractionation of the Absheron reservoir in the apparatus of "Crude Oil Distillation" for the purpose of the establishment of the true boiling temperature curves and the acquisition of commodity and fat fractions, fuel, kerosene and diesel fuel based on narrow fractions fractions were prepared and their quality and group hydrocarbon composition was determined. It was determined that c. 85°C, as a component of the car gasoline, for the fractional catalytic reforming process of 85°C to 180°C, lightweight kerosene fractions TS 1 and Jet A 1 jet fuel, diesel fractions D 02, winter and summer diesel fuel was offered as raw material. The main quality indicators of commodity fractions have been studied in accordance with international standards and have been found to be of the same quality. Distillate oils from the distillate fractions of Absheron cube in the range 300-500°C, with distillate oils of 27.12%, viscosity indexes 23.5 to 43.0, and from 500°C to 10.9% oil is obtained. The Absheron Cube is 100 g at 260°C in the laboratory device to obtain bitumen from commercially available oils (500°C). 0.2 I / min to the residue. oxidation was carried out by the air, and as a result bitumen was obtained, meeting BNB 70/30 construction bitumen standard requirement by road bitumen BNB 50/70 and oxidation for 14 hours. Absheron cube oil is a good raw material for gasoline, various jet and diesel fuel, oil and bitumen.

# THREE-, TWO-, AND ONE-PHASE ISOCHORIC HEAT CAPACITIES AND PHASE TRANSITION IN *I*/-HEXANE + IL MIXTURE NEAR THE CRITICAL POINT OF PURE *I*/-HEXANE

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Isochoric heat capacity of binary n-hexane+IL (1-octyl-3-methylimidazolium chloride, abbreviated as [C<sub>8</sub>C<sub>1</sub>Im]<sup>+</sup>[CI]) along the fixed isochore of 255.19 kg·m<sup>-3</sup> as a function of temperature near the critical point of pure solvent (nhexane) were measured. The measurements were performed for the selected concentration of 0.0089 mole fraction of IL in the three- (L-L-V), two- (L-V), and one (L) -phase regions over a temperature range from (308 to 527) K at pressures to 4 MPa. The measurements were performed using a high-temperature, high-pressure, nearly constant-volume adiabatic calorimeter. The combined expanded uncertainty of the density, temperature, concentration, and isochoric heat capacity, C<sub>v</sub>, measurements at the 95 % confidence level with a coverage factor of k = 2 is estimated to be 0.15 %, 15 mK, 0.0001, and 3 %, respectively. The possibility of the chemical reactions occurring during heat capacity measurements at high temperatures has been discussed. The onset of the effects of thermal decomposition (chemical reaction) on the isochoric heat capacity of *n*-hexane+IL mixture was found at temperatures above approximately 429 K. The addition of *n*-hexane into the IL made little change its thermal stability. The L-V phase-transition parameters ( $T_s$  =509.88 ±0.05 K,  $\rho_s$  =255.19 kg·m<sup>-3</sup>, and  $P_s$  =3.1175 MPa) have been measured using heat capacity abrupt behavior. Addition of the IL (0.0089 mole fraction of IL) shifts (increases) the phase-transition (critical) temperature of pure *n*-hexane by 2.058 K, while the critical temperature increases by 0.8755 MPa. As a test measurement the isochoric heat capacity of pure *n*-hexane along the selected near-critical isochore ( $\rho_s$  =245.67 kg·m<sup>-3</sup>) in the two- and one-phase regions have been measured. The measured phase transition parameters ( $T_s$  =507.71 ±0.05 K,  $\rho_s$  =245.67 kg·m<sup>-3</sup>, and  $P_s$  =3.041 MPa) for pure *n*hexane are in good agreement with reference data (REFPROP/NIST).

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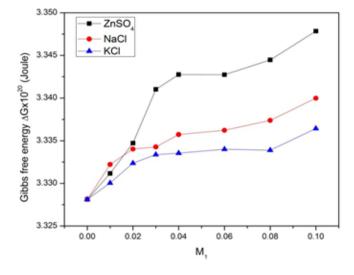
# DENSITY, ULTRASONIC VELOCITY, VISCOSITY, REFRACTIVE INDEX AND SURFACE TENSION OF AQUEOUS CHOLINE CHLORIDE WITH ELECTROLYTE SOLUTIONS

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Choline Chloride being a quaternary ammonium salt, non-toxic and biodegradable compound, it has been studied as deep eutectic solvents (DES). It also plays vital role in neurotransmission, normal cell functioning and as a dietary component. It is widely used as a nutritional additive in livestock.

The present studies give density, viscosity and ultrasonic velocity measurements for mixtures of aqueous Choline Chloride with three different electrolytes (ZnSO<sub>4</sub>, NaCl & KCl) under atmospheric pressure at various concentrations and 298.15 K. Refractive index measurements have been carried out at five different temperatures ranging from 308.15 to 328.15 K with 5 K difference. Thermodynamic and thermophysical parameters like isentropic compressibility ( $\beta_s$ ), acoustic impedance (Z), intermolecular free length (L<sub>f</sub>), relative association (R<sub>A</sub>), viscous relaxation time ( $\tau$ ), Gibbs free energy ( $\Delta$ G), surface tension ( $\sigma$ ), free volume (V<sub>f</sub>) and internal pressure (P<sub>i</sub>) have also been evaluated. The findings have been utilized to understand the presence of solute-solvent



interactions and the structural effects on the solvent in solutions to analyse the molecular interactions prevalent in the systems. The viscosity measurements were correlated with the Jones Dole coefficients and the interactions have been explained based on Kosmotropic and Chaotropic behaviour.

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# THERMODYNAMIC PROPERTIES OF GRAPHENE SHEET DEPOSITED ON POLAR CRYSTALLINE MATERIAL

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In recent times there has been a focus to developing nanosensors using thermodynamic properties of graphene nanocomposites in crystalline materials [1-3]. Here we present the effect of thermal conduction and external laser on a nanocomposite system composed of metallic graphene sheet and a polar material such as SiO<sub>2</sub>. Such systems are fabricated by depositing graphene sheet on a polar crystallin substrate. These systems have the luxury of having four quantized particles such as phonons, plasmons, polaritons and surface plasmon polaritons. These particles interact with each other. Thermal phonons in the polar material couple with surface plasmons of the graphene sheet which in turn produces new particles called phonon plasmon polaritons (PPPs). Similarly, photons from the external laser couple with surface plasmons of graphene sheet to form surface plasmon polaritons (SPPs). We consider that the excitons in the QD interact with the PPPs and the SPPs of the hybrid system. Using Maxwell's equations in the quasi-static approximation the polarizability of the graphene sheet is calculated. The temperature dependence thermal conduction is calculated by using the Kubo formulism. The absorption and emission of the graphene is calculated the density matrix method. For this hybrid system we performed numerical simulations on thermal and electrical properties of the nanocomposite. We have found that when PPPs and SPPs energies have same energy as the graphene band gap the absorption peak splits into two peaks due to PPPs and SPPs couplings. In the same time, it is also found that thermal conduction also increases due to PPP and SPP couplings. The thermal and electrical energy transfer from the polar material (SiO<sub>2</sub>) to graphene sheet can be controlled by applying thermal pressure in the system. The splitting of the one peak to peaks can also be controlled by the thermal pressure or temperature gradients. These findings can lead to the fabrication of temperature and pressure sensors in the THz range.

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# **Company Presentation**



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Anton Paar GmbH is an Austrian company with its registered office in Graz that develops, produces and sells analytical instruments for laboratories and process analysis technology (PAT). It also supplies customised automation and robotics solutions. The company is specialised in the production of equipment for measuring density and concentration and in rheometry and the determination of dissolved carbon dioxide CO<sub>2</sub>.

Anton Paar GmbH manufactures at its site in Graz and has five other manufacturing subsidiaries in Austria, Bosnia, Germany and Switzerland. Worldwide, there are 26 sales subsidiaries and numerous international sales partners.

The company Anton Paar is committed to long-term partnerships with customers and employees as well as responsibility towards society in general. Since 2003 Anton Paar has been owned by the charitable Santner Foundation. The foundation is exclusively and directly dedicated to charitable and beneficent causes.

Over 2500 employees at the headquarters in Graz and the 26 sales subsidiaries worldwide ensure that Anton Paar products live up to their excellent reputation. The core competence of Anton Paar – high-precision production – and close contact to the scientific community form the basis for the quality of Anton Paar's instruments.

Ninety-three per cent of the products from the globally active measuring technology manufacturer are exported to more than 110 countries around the world.

Around 20 per cent of the annual turnover of Anton Paar GmbH is invested in research and development in order to development new measuring principles, sensor generations and technology concepts.

# Products of Anton Paar GmbH

Core areas - measurement, analysis, chemical synthesis:

- Fusion equipment for chemical analysis and synthesis: Anton Paar develops and produces equipment that prepares, extracts and synthesises samples with the assistance of microwaves.
- Automation & Robotics: Anton Paar offers fully automatic sample handling for all requirements of analysis with a high sample throughput and to monitor production processes.
- Measurement of density and concentration: Anton Paar measuring devices are used to determine the density and concentration of liquids, e.g. in product development, quality assurance and in checks during production, for instance in the food and beverages industry. Anton Paar is the global market leader with its measuring equipment for the quality control of drinks. In 1967, Anton Paar launched the world's first digital density measuring device on the market.
- Petroleum analysis: Anton Paar develops and produces petroleum testing devices that analyse the properties of petroleum and petroleum products such as the flashpoint, the distillation curve, corrosiveness, oxidation stability, cold properties, consistency or ductility.
- Microwave technology for chemical analysis and synthesis
- Testing of micro and nano hardness, checking for cracks, and measurement of layer thickness

- Raman spectroscopy: In December 2016, Anton Paar acquired a product line from the field of Raman spectroscopy as well as licensed handheld Raman technology from the US. Raman spectrometers are measuring devices that record a chemical fingerprint of the molecules of liquids and solids.
- Refractometers and polarimeters: Refractometers determine concentrations in liquids; polarimeters measure the optical rotation. The measuring instruments are used in the quality control of pharmaceutical active ingredients and foods.
- Systems for X-ray structure analysis: Anton Paar produces systems for the material characterisation using X-ray small-angle scattering and measuring chambers for X-ray diffraction. The company entered the field of X-ray structure analysis in the 1950s when it commenced collaboration with Prof. Otto Kratky. The first X-ray small-angle cameras were developed further by Anton Paar into complete systems that today are used in research and teaching, in the field of life science and material sciences.
- Particle and surface characterisation: With the Anton Paar "Litesizer" measuring instruments, the particle size and zeta potential in liquids is determined by dynamic light scattering. The stability of particle dispersions and emulsions is thus analysed and the charging of surfaces determined.
- Process analysis technology: Process analysis technology from Anton Paar is used by plant operators in the food and beverages industry, petrochemical and chemical industry. Density of liquids and gases, concentration of substances dissolved in liquids, dissolved oxygen and dissolved carbon dioxide are determined by highly precise sensors.
- Viscosimeters and rheological measuring instruments: viscosimeters determine the viscosity (ductility) of liquids and semi-solid products at different temperatures. Rheometers measure the visco-elastic characteristics of fluid and malleable materials.

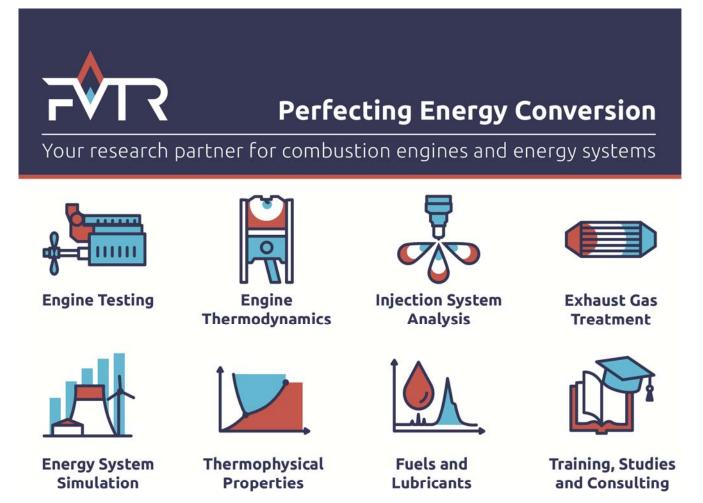
# Anton Paar's product portfolio for thermophysical measurement includes:

Density meter for high temperature and high pressure DMA 4200 M and DMA HPM measure the density of liquids and gases up to a temperature of 200°C and 1400 bar. These density meters are used for the determination of equation of states and pVT- studies.High Precision Thermometers



 The MKT 50 Millikelvin Thermometer is designed for the most accurate temperature measurements, comparison calibrations and fixed point calibrations. The MKT 10 is the small "brother" of the MKT 50 and gives accurate temperature measurement with a measuring uncertainty of 10 mK.





As an independent development service provider in the fields of thermal processes and machines, we contribute to the product development chain at the interface of fundamental university research and the specific requirements of business enterprises.

At the core of our work is the experimental and simulation based analysis of energy conversion processes in mobile and stationary applications – ranging from automotive and ship propulsion up to thermal power plants. Beyond that, we are eager to investigate all the underlying phenomena involved and to collaborate with the adjoining technology sectors to leverage all imaginable potentials. One of our main goals is to contribute to the technical advancement of thermal based machines. Not for the sake of it but because we are highly convinced that thermal machines will continue to play a significant role in the future of energy supply and because we see the potential in this technology in our every day's work.

We are really looking forward to assist you during the realization process of your ideas and products.



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high precision thermoregulation



# Peter Huber Kältemaschinenbau AG

#### Company Profile

Huber Kältemaschinenbau is the technology leader for high precision thermoregulation solutions in research and industry. Our products ensure precise temperature control in laboratories, pilot plants and production processes from -125°C to +425°C. The company employs approximately 300 employees at its headquarters in Offenburg and operates internationally with offices and trading partners. More than 250,000 Huber temperature control products are in use in science, research and industrial applications. In 2018 Huber was awarded with the "TOP 100 Innovator" seal for being one of the most innovative medium sized companies in Germany.



#### History

Huber Kältemaschinenbau was founded in 1968 as one of the first companies in refrigeration systems. Huber has pioneered the technological development in the field of fluid temperature control with several innovative products. A revolution in temperature control technology was the introduction of the Unistat temperature control systems in 1989. Even today Unistats set the tone when it comes to highly dynamic temperature control processes. Typical applications can be found in process engineering, the semi-conductor industry, solar technology industries, materials testing as well as research in the chemical, pharmaceutical and petro-chemical industries. Apart from the Unistat systems the product range includes chillers, heating and cooling circulators, visco baths, calibration units and a wide range of customized solutions.

#### Products

The Huber product range offers solutions for all temperature applications from -125 °C to +425 °C. The range includes highly dynamic temperature control systems with cooling capacities up to 250 kW as well as chillers and heating and cooling thermostats for applications in laboratory, pilot plant and production.

#### Dynamic Temperature Control Systems – Unistat®, Tango®, Grande Fleur®, Petite Fleur®

- Huber Unistat offer unmatched thermodynamics and advanced control technology.
- Efficient heating and cooling technology
- Short heating and cooling
- Wide temperature range with no fluid exchange
- More than 60 models with cooling of 0.7 to 130 kW

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- Circulators for external temperature
- Refrigeration and Low Refrigerated Circulators
- Over 70 models with cooling capacities up to 7 kW

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- Huber Minichiller and Unichiller offer environmentally friendly and economic cooling solutions.
- Environmentally friendly alternative to cooling with fresh water
- Small size, high performance
- Rugged stainless steel construction
- Proven, reliable technology life
- Over 50 models with cooling capacities from 0.3 to 50 kW

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hydroforming presses, chemical industry and systems for institutes of universities or research & development departments.

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Dieckers is a member of the working group water jet technology (AWT) of the university of Hannover, which was founded in 1991 to develop applications for industries as well as for research and development. Actually there are 80 partners from nine countries that are members of the AWT.











#### IXUN Lasertechnik GmbH

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With know-how and long-term experience in the sector of surface processing with laser radiation, IXUN offers individual solutions for processing single and series-produced components.

IXUN also produces customized inner and outside cladding optics for industrial use. As a spin-off of the Fraunhofer ILT with headquarters in its Application Center, the most modern laser and handling systems are available to IXUN Lasertechnik GmbH.

#### **IXUN PRODUCTS**

IXUN develops and builds customer-specific inner and outside cladding optics, as well as powder and protective gas nozzles for all laser beam sources. IXUN optics can be customized individually regarding to laser beam source, insertion depth and workable internal diameter. They are suitable for conventional as well as for high-speed laser welding.

#### IXUN optics have been proven for years in intensive industrial use and are characterized by: Our Optics

- Matched focus shape round, linear or rectangular
- Variable external diameter
- Variable insertion depth
- Variable internal diameter starting from 25mm
- · Horizontal and vertical processing possible
- With multi-beam, off-axis or coaxial nozzle
- · Suitable for high-speed laser welding
- Durability up to 6 KW laser power

#### Our Strength: Inner Cladding Optics (IXUNClad®)

IXUN optics are suitable for both internal and external processing, for laser hardening, coating, dispersing, welding or alloying.

The optics have been proven for years in intensive industrial use.

#### **RANGE OF SERVICES:**

The laser offers a wide range of possibilities for repair as well as wear and corrosion protection of components, which cannot be realized with any other technology.

#### Advantages of laser processing

- Layers from 0.1 mm to several cm
- · Metallurgical bonding of the layers

- · Low heat input and therefore lower distortion
- Processing of almost all metal alloys
- Large selection of filler materials
- High precision of the deposited layers
- Repair of polished surfaces
- Processing of 3D contours
- Cladding of critical positions (cast channels, sealing edges or cooling channels)



#### Advantages for you as a customer

- Saving replacement costs
- Reduced machine downtimes
- · Increased wear resistance
- Modification/repair instead of new production
- Preservation of unique parts, e.g. vintage car parts
- Repair of parts that cannot be repaired with conventional techniques

#### Our range of services:

- Laser processing of inner and outer contours with:
- Laser cladding
- Laser alloying and dispersing
- Laser heat treatment (hardening, tempering, stress-free annealing)
- High-speed laser welding
- · Processing of single- and series-produced parts
- · Feasibility studies
- · Development of customized inner cladding optics
- Development of customized outside cladding optics
- Development of customized powder feed and protective gas nozzles (off-axis, multi-beam and coaxial)
- Implementation and process optimization

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- Die casting tools
- Forging tools
- Forming tools
- Fixtures

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- · Motor blocks, cylinder heads
- Pistons, valve, valve seats
- · Gearbox components (bearings, casings)

#### General mechanical engineering

- Containers
- Running wheels
- Gear racks
- Shafts
- Extruder screws
- · Components from the oil and gas industries

Leybold

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# Innovative Vacuum Components and Systems for Versatile Applica-

Consulting, sales and service Single-stage rotary vane pumps Dual-stage rotary vane pumps **Diaphragm pumps** Oil-free scroll pumps Dry compressing multi-stage roots pumps Dry compressing screw pumps and systems Dry compressing screw pumps Roots blowers Oil vapor jet pumps Oil diffusion pumps Control unit for oil diffusion pumps and OB pumps Turbomolecular pumps with hybrid bearing technology (mechanical/ma Turbomolecular pumps, magnetically levitated Turbomolecular pumps, magnetically levitated Refrigerator cryo pumps Cold heads for cooling cryo pumps/cryostats Vacuum gauges and pressure gauges Vacuum controller Leak detectors and leak testing systems Central vacuum stations Multistage forevacuum systems Experimentation and coating systems Custom vacuum calibration systems Innovative pump and system management High vacuum pump systems Valves in different design types and driving modes Connection components Vacuum oil, pump fluids and special lubricants









# Swagelok Leipzig | Berlin

#### QUICK FACTS

- Ranked among top private companies
- Approximately \$1.5 billion (USD) in annual sales
- 4,000 associates worldwide
- Worldwide manufacturing, distribution, and technical centers
- Sales focused by market and by region





#### LOCAL SERVICE

- Located in 57 countries on six continents
- Familiar with local languages, customs, and business practices
- Provide excellent on-site service and training

#### MARKETS SERVED

- Alternative fuels
- Biopharmaceutical
- Chemical and petrochemical
- Food, beverage, and dairy
- Oil and gas
- Power
- Pulp and paper
- Semiconductor
- Shipbuilding

### UNIQUE BUSINESS MODEL

- Over 200 authorized Swagelok sales and service centers worldwide
- 3,000 sales and service associates
- 6 sales and service center in Germany

Swagelok sales and service center in eastern Germany,

21 sales associates located in Leipzig, Branch office Berlin, 9 sales associates service area eastern Germany



#### **GLOBAL REACH**

- Technical and distribution centers deliver solutions around the world
  - Lachen, Switzerland
  - Osaka, Japan
  - Pune, India
  - Shanghai, China
  - Solon, Ohio

#### **EXPANDED SERVICES**

- We provide many services to meet a variety of customer challenges
  - Swagelok® Custom Solutions
  - Design and engineered-to-order services
  - Energy conservation services
- Education services
- Transaction services
- Technology services

#### QUALITY CERTIFICATIONS AND COMPLIANCE

- Lloyd's Register of Shipping (LRS)
- United States Department of the Navy
- ECE/R110 for components in compressed natural gas vehicles
- ASTM F-1387 for performance of mechanically attached fittings
- CRN (Canada)
- Vd TÜV (Germany)
- ASME N and NPT certificates nuclear safety-related applications (U.S.A.) improves productivity
- European Pressure Equipment Directive (PED)
- METI/KHK (Japan)
- Det Norske Veritas (DNV)
- Nippon Kaiji Kyokai (NK)
- American Bureau of Shipping (ABS)

#### **INNOVATIVE PRODUCTS**

- New product development
- Continued refinement and adaptation of existing designs
- Engineered-to-order products and custom configurations
- Solutions, including custom fabrications, subassemblies, and training
- Over 200 patents in force worldwide



#### **PRODUCT BREADTH**

- Over 290,000 end item product variations
- 7,000 parts stocked globally
- Filters
- Fittings
- Hoses
- Measurement devices
- Tubing and tube supports
- Valves
- Welding systems
- Regulators
- Sample cylinders
- Miniature modular systems
- Quick connects

#### VALUE IMPACT PARTNERSHIP

- Systematically calculates the financial value of our Swagelok's services
- Itemized statement includes:
  - Consignment
- eBusiness solutions
- Emergency delivery
- Energy management
- Engineering services
- Equipment services
- Custom solutions
- Just in time delivery
- Kitting
- Product evaluations
- Summary billing
- Steam audits and training
- Swagelok weld system training
- Vendor managed inventory



• Thermtest Inc. Fredericton, NB, Canada

+1 506 458 5350 info@thermtest.com | Thermtest.com

#### **COMPANY PROFILE:**

Thermtest is a leading international developer of thermal instruments and testing services for clients over a broad range of industries and international markets. They design, manufacture and distributes testing instruments that measure thermal conductivity, thermal diffusivity, thermal resistivity, thermal effusivity, specific heat capacity and thermal analysis. The company's thermophysical testing lab and R&D facility is in its headquarters in New Brunswick, Canada with hubs in Europe and Latin America.

#### **HISTORY:**

Thermtest was incorporated in 2005 as one of the first companies in Canada that designs, manufactures, and distributes thermal measurement instruments worldwide. In 2018, Thermtest opened its first international location "Thermtest Europe AB" in Sweden. For the past 15 years, Thermtest has operated a world-class testing services laboratory, featuring more than 10 thermal conductivity methods. The invaluable experiences and knowledge gained daily, coupled with the ongoing collaboration with our customers and business partners, fuel our successes and passion to continue to expand and improve upon our full spectrum of innovative thermal conductivity technologies as we look to the future.

#### PRODUCTS LABORATORY EQUIPMENT



HFM-100 Materials: Insult

Materials: Insulation, Solids, and Textiles Property: Thermal Conductivity Method: Heat Flow Meter Standard: ASTM C518, ISO 8301, and EN 12667



THW-L1 Materials: Liquids and Pastes Property: Thermal Conductivity, Thermal Diffusivity and Specific Heat Methods: Transient Hot-Wire Standard: ASTM D7896-19



# DSC-L600

Property: Thermal Analysis Methods: Differential Scanning Calorimetry Standard: Conforms to ISO and ASTM standards



TGA-1000/1500 Property: Thermal Analysis Methods: Thermogravimetric Analysis Standard: Conforms to ISO and ASTM standards



#### PORTABLE METERS

TLS-100 Materials: soil, rocks, concrete, and polymers Property: Thermal Conductivity, Thermal Resistivity Methods: Transient Line Source Standard: ASTM D5334-14

THW-L2



Materials: Liquids and Pastes Property: Thermal Conductivity Methods: Transient Hot-Wire Standard: ASTM D7896-19

#### GHFM-02

Materials: Metals, Polymers and Composites Property: Thermal Conductivity and Thermal Resistance Methods: Guarded Heat Flow Meter Standard: ASTM E1530-19



#### TPS-EFF

Materials: Textiles, Fabrics and Solids Property: Thermal Effusivity Methods: Transient Plane Source Standard: ASTM D7984-16 www.imspolymers.com

# **R&D** Center

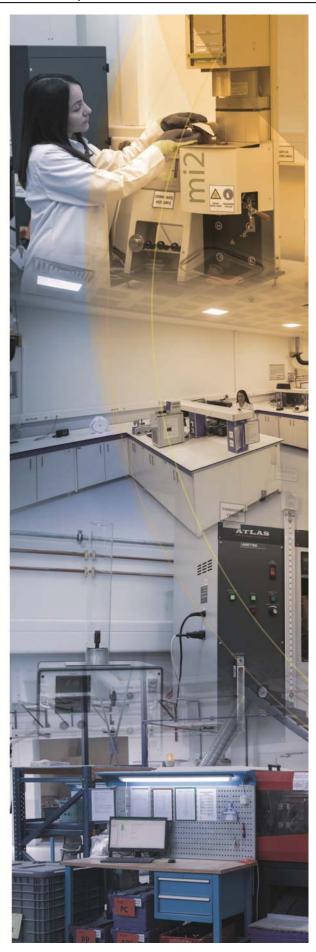
In January 2015, IMSPolymers established a research and development office in Ege University's IDEEGE Technopark to develop the university-industry business association. After the product development studies started on an academic basis, the production plant located in the 1st Organized Industrial Zone of Turgutlu, Manisa, has been in production since October 2015.

IMSPolymers, thanks to its vision, has entered among the major players in the market. Established fully with domestic capital, IMS Polymers has been recently approved as an R&D center on October 5, 2017 by the "Ministry of Science, Industry and Technology". Within the R&D Center; there are 3 part-time (1 professor, 2 associate professors), 2 support and 17 full-time R&D working staff.

Efforts to develop functional and value-added engineering plastics for many sectors including energy, electrical and electronics, construction, automotive, biomedical and railway are being pursued with both owner's equity and project support. The R&D Center has a state-of-the-art 205 m<sup>2</sup> test laboratory and production area, 150 m<sup>2</sup> R&D central office, with total closed area of approximately 670 m<sup>2</sup>.

Value-added product development projects, accelerated by technological developments are carried out meticulously considering the needs of the market. Within this context, as of 2016, "Graphene Reinforced Polymeric Composite Compact Heat Exchanger Design and Production" named San-Tez project and at the end of 2017 "Development of Polypropylene Composites with Halogen-Free Flame Retardant Properties" titled Tübitak 1507 project, were completed. Employees of the R & D center continue to make contributions to the literature through the papers and scientific publications that have emerged as a result of successful projects. At the R & D Center; Tübitak Teydeb (1501, 1507, 1511), Ardeb 1003 and Tübitak 3501 projects are successfully being carried out.

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Analytik Jena is a leading provider of high-end analytical measuring technology, of instruments and products in the fields of biotechnology and molecular diagnostics, as well as of high quality liquid handling and automation technologies. Its portfolio includes traditional analytical technology, particularly to measure concentrations of elements and molecules, as well as systems for bioanalytical applications in the Life Science area spanning the highly complex analytic cycle of a sample from sample preparation to detection. Automated high-throughput screening systems for the pharmaceutical sector are also part of this segment's extensive portfolio. Analytik Jena's products are focused to offer customers and users a quality and the reproducibility of their laboratory results. Services, as well as device-specific consumables and disposables, such as reagents or plastic articles, complete the Group's extensive range of products. Analytik Jena is part of the Swiss Endress+Hauser Group.



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