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Book of Abstracts

THERMAM 2018

7th Rostocker International Conference:
“Thermophysical Properties
for
Technical Thermodynamics”

Institute of Technical Thermodynamics

University of Rostock,
Rostock, Germany

26 – 27 July, 2018

THERMAM 2018

7th ROSTOCKER INTERNATIONAL CONFERENCE: "THERMOPHYSICAL PROPERTIES FOR TECHNICAL THERMODYNAMICS"

26 - 27 July 2018

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Density measurements up to 4000 bar and temperatures up to 200 °C

Density measurements at ambient pressure and various temperatures

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

Vapor pressure measurements at high temperatures

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

Vapor pressure measurements at small temperatures

BOOK OF ABSTRACTS

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Albert Einstein Str. 2,
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Preface

7th ROSTOCKER INTERNATIONAL CONFERENCE ON THERMOPHYSICAL PROPERTIES FOR TECHNICAL THERMODYNAMICS

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 in the atmosphere clearly have to do with 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 thermodynamics problems one needs “Thermophysical and Mechanical Properties of Advanced Materials”. One example is the possible capture of carbon dioxide from atmosphere or exhaust gases in ionic liquids. To make this technically feasible data for the thermophysical property of solution of carbon dioxide in the advanced material of an ionic liquid are needed.

Within 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.

We choose the venue of the conference as the exciting city of Rostock with all the amenities of such a place in a very nice surrounding and with the possibility to explore the old and new city and even excursions to historically interesting tourist sites like Old City, Warnemünde etc.

We wish you a very pleasant, joyful, interesting and stimulating conference at the Rostock University, GERMANY.

THE ORGANIZING COMMITTEE

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Keynote Presentations

DENSITY AND DERIVATE THERMODYNAMIC PROPERTIES OF 1-ETHYL-3-METHYLIMIDAZOLIUM METHANESULFONATE+METHANOL BINARY MIXTURES AT HIGH TEMPERATURES AND HIGH PRESSURE

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Prof. Dr.-Ing. habil. Dr. h. c. Egon HASSEL is Professor and chair of Technical Thermodynamics at the University of Rostock in Germany since 1999. He studied physics at Technical University of Aachen, Germany, and went early into Mechanical Engineering, where he received his PhD at Technical University of Aachen and later his Habilitation at Mechanical Engineering from Technical University of Darmstadt, Germany. His interests mainly cover the fields of energy technique, IC engine combustion and measurements of thermodynamic properties. In November 2012 he received an honorary doctorate from Azerbaijan Technical University in Baku.

Ionic liquids (ILs) are received wide range of application in industry at last decades as heat transfer fluids in absorption refrigerating and solar heating systems, in separation technologies, as liquid crystals, templates for the synthesis of mesoporous, nanomaterials, *etc*. Accurate knowledge of the thermodynamic properties of ILs is required to improve the technologically important applications of ILs and develop accurate equation of state. In the present work the density of [EMIM][MeSO$_3$] and methanol binary mixtures at high temperatures (from 273 to 413 K) and high pressures (up to 60 MPa) were measured using the Anton-Paar VTD DMA HPM. The combined expanded uncertainty of the density, ρ, pressure, P, and temperature, T, measurements at the 95 % confidence level with a coverage factor of k = 2 is estimated to be (0.01 to 0.08) % depending on temperature and pressure ranges, 0.1 %, and 15 mK, respectively. The present work is considerable expanding the available thermodynamic database for the [EMIM][MeSO$_3$] +methanol binary mixtures to high (to 413 K) and low temperatures (to 273 K) and high pressure (to 60 MPa).

In addition the speed of sound and heat capacity of the mixture at atmospheric pressure were measured using a sound-speed analyzer (Anton Paar VTD DSA 5000 M) and DSC Pyris-1 in the same temperature range. The measured high-pressure *PVT* data were used to develop polynomial type multiparametric equation of state. This equation of state together with measured heat capacity values at atmospheric pressure was used to calculate other derived thermodynamic properties such as isothermal compressibility $\kappa_T(p,T)$, isobaric thermal expansibility $\alpha_p(p,T)$, thermal pressure coefficient $\gamma(p,T)$, internal pressure $p_{int}(p,T)$, specific heat capacities $c_p(p,T)$ and $c_v(p,T)$, speed of sound $u(p,T)$, isentropic expansibilities $\kappa_s(p,T)$ at high temperatures and high pressures, in which the (p,ρ,T) data of [EMIM][MeSO$_3$] and methanol mixtures were measured. The excess molar and apparent molar volumes of the mixtures were calculated using the pure components and mixture property data.

APPLICATION OF ACOUSTIC METHOD FOR DETERMINATION THERMOPHYSICAL PROPERTIES OF IONIC LIQUIDS FOR THEIR USE AS HYDRAULIC FLUIDS

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Prof. Marzena DZIDA is Professor and a Head of Department of Physical Chemistry and a Vice-Director for Research of Institute of Chemistry of University of Silesia in Katowice. She is interested mainly in application of the acoustic methods in determining thermodynamic properties of the liquids, especially ionic liquids and biofuels under high-pressure, thermophysical properties of IoNanofluids, description relationships between chemical structure of the liquid state and physicochemical properties, development of the apparatuses for the speed of sound measurements.

Only a fluid with low compressibility and optimal lubricity is able to transfer pressure in the system without delay and low energy losses due to compression of the fluid itself. Hydraulic fluids should also have a low vapour pressure and low gas solubility, which causes that at high temperatures there is no gas that would significantly increase the compressibility of the system. Ionic liquids are currently subject of intensive research as friendly environmental engineering solvents and working fluids. Ionic liquids have relatively low saturated vapour pressure at high temperatures, low compressibility and thermal expansion, which predates them as good candidates as hydraulic fluids. The investigations of the speed of sound in ionic liquids are undertaken among others to obtain key thermophysical properties for their use in chemical and industrial processes. The only experimental method that leads directly to isentropic compressibility is the acoustic one, based on the measurement of the speed of sound. The knowledge of the isentropic compressibility allows for the most accurate and the most convenient way to determine the related thermophysical properties of the liquid phase at atmospheric or at high pressures. In particular, it allows to calculate the isothermal compressibility of liquids. The thermophysical properties of compressed thiocyanate- and ethyl sulfate-based ionic liquids have been studied in order to applied them as hydraulic fluids. Thermophysical properties under high pressures up to 100 MPa was determined by the acoustic method. The temperature and pressure ranges of speed of sound measurements were chosen carefully because the pressure-temperature investigations of the thermodynamic properties using the acoustic method must be carried out outside of the dispersion region. The high pressure thermophysical properties, especially isobaric thermal expansion and isothermal compressibility of studied ionic liquids are compared with the reference mineral, synthetic, and biodegradable oils as well as commercial hydraulic oils. In the age of advanced technologies development, the ethyl sulfate-based ionic liquids could be used in industry in a large scale as hydraulic fluids, considering the fact that they have more advantages than disadvantages.

UNDERSTANDING TRANSITION ENTHALPIES OF IONIC LIQUIDS AT THE MOLECULAR LEVEL

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Prof. Dr. Ralf LUDWIG is Professor and Head of Physical Chemistry at the University of Rostock, Germany. His major research activities are in the field of clusters, liquids and solutions. The main goal is to predict macroscopic properties on the basis of molecular interactions. Currently, he serves as editorial board member for „Zeitschrift für Physikalische Chemie" and for „Scientific Reports". Since 2016 Ludwig is also member of the Fachkollegium FK 303 „Physical and Theoretical Chemistry" of the German Science Foundation (DFG).

Understanding transition enthalpies of ionic liquids is challenging. In this talk, we show that spectroscopy, quantum chemical calculations and molecular dynamics simulations allow an interpretation of these thermodynamic properties at molecular level. Here, we will address a number of relevant questions. What are the structures present in the solid state, in the liquid or in the gas phase? How are these specie characterized by the subtle balance between Coulomb interaction, hydrogen bonding and dispersion forces?

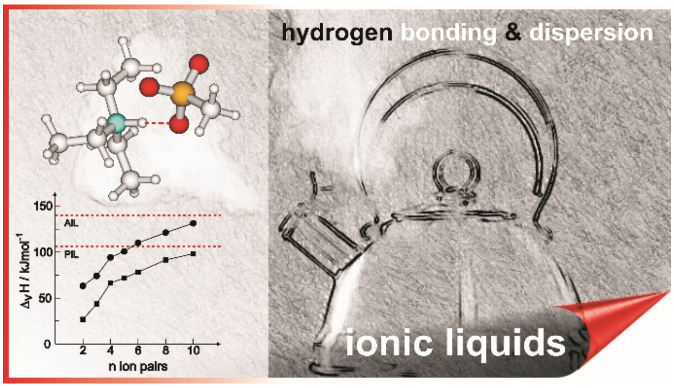

Figure: Vaporization enthalpies are higher for aprotic ionic liquids than that for protic ionic liquids.

Why is the vaporization enthalpy for ethyl ammonium nitrate high but the boiling point so low? Why are the vaporization enthalpies of aprotic ionic liquids significantly larger than that of protic ionic liquids? How are the transition enthalpies between contact and solvent separated ion pairs governed by temperature, solvent polarity and solvent concentration? How large is the transition enthalpy, which is required to shift the equilibrium from H-bonded to dispersion-driven cation-anion interaction? Does like-charge attraction affect the solid-liquid phase transition?

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HEAT TRANSFER IN SUPERCRITICAL FLUIDS: RECONCILING THE RESULTS OF FAST AND STATIONARY MEASUREMENTS

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Prof. Pavel V. SKRIPOV is Professor of the Ural Institute of State Fire Service of EMERCOM of Russia, leading researcher of the Institute of Thermal Physics, Ural Division of Russian academy of sciences. He has developed new approaches for studying pulse-heated liquids in short-lived states which are of interest from both fundamental and practical considerations. Using novel experimental methodology combined with the original in-house hardware and software solutions, his research team obtained robust experimental results describing thermophysical properties and heat transfer in superheated liquids and supercritical fluids under high-power heating regimes.

Our report deals with the essential features of heat transfer in supercritical fluids (**SCFs**) at different temporary and spatial scales of the system. Due to the anomalous behavior of thermophysical and kinetic properties of a substance in the near-critical region, SCFs have indeed attracted significant attention, in particular, in relation with the prospective nuclear power program [1]. By the sum of factors, this region is referred to as “a very delicate state of matter” [2]. From the point of view of experimentalists, this feature leads to the strict requirements to both the procedure of determining the primary values from the measurements and the interpretation of the results obtained on their basis. In this connection, we will consider in detail the pioneering investigations of the heat transfer and thermophysical properties of fluids in the near-critical region, see, for example, refs. [3, 4]. The results of these studies have formed a basis for a great progress in understanding the critical phenomena and assessing their prospects for engineering applications.

In terms of a discussion, these results, stationary by their very nature, will be complemented by those obtained by the method of controlled pulse heating of a fast-response wire probe, which has been developed by us. The characteristic heating time is a few milliseconds, and the heat flux density through the probe surface is increased up to 10 MW/m^2. For all substances studied, the stepwise decrease in the heat transfer intensity has been revealed in the course of crossing the vicinity of the critical temperature along the isobar [5, 6]. This contradicts the heat transfer pattern typical of the stationary case. The essential point is that the short duration of observation of the supercritical state and, correspondingly, the small thickness of the heated layer allow us to exclude from consideration the convective instability and gravitational sensitivity in the near supercritical region. These two features characteristic of SCFs are the key factors that call for a re-examination of the results of thermal conductivity measurements performed in stationary conditions. The final solution of the problem of reconciling the pulse heating results with the peaks of thermophysical properties derived from stationary experiments in the near-critical region has not been found so far.

This study was supported by the UB RAS Complex Program (grant no. 18-2-2-3).

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NEW METHOD FOR THE ESTIMATION OF TRANSPORT PROPERTIES OF ELECTROLYTES USING MODIFIED UNIFAC-BASED MODELS

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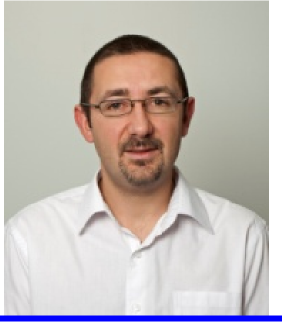
Dr. Johan Jacquemin is has expertise in the development of in-house property databanks, the design of novel and original experimental apparatus and physical models able to predict properties with a view to understanding the physical and chemical nature of novel materials and design of viable chemical engineering process. He passed with honours a PhD investigating thermodynamics of selected Ionic Liquids in July 2006 at the University Blaise Pascal (Clermont-Ferrand – France). He has published > 120 peer reviewed journal papers (h-index 29). He has supervised more than 20 Master Students, 8 MPhils and 12 PhD students.



Modified UNIFAC-VISCO [1-2] and UNIFAC-CONDUCTIVITY [3] group contribution methods were developed for the correlation and estimation of the transport properties of a series of electrolytes as a function of temperature and composition at 0.1 MPa using a large set of recommended data from the literature. During this work, experimental data were critically assessed using the statistical method and mathematical gnostics to highlight recommended data used then to develop the modified UNIFAC-based models.[1-2] In this original approach, exemplified in Figure 1 in the case of the viscosity of pure ionic liquids, the salt (ionic liquids and/or molten salts) was divided into two peculiar function groups, cation and anion. Binary interaction parameters were determined by fitting the recommended experimental data and by minimizing the objective function. The transport properties of cations, anions, and salts showed an exponential behavior with the temperature well described thanks to the Vogel-Fulcher-Tamman (VFT) equation. Calculated VFT constants and binary interaction parameters were used to evaluate the viscosity, conductivity and ionicity of selected electrolytes.

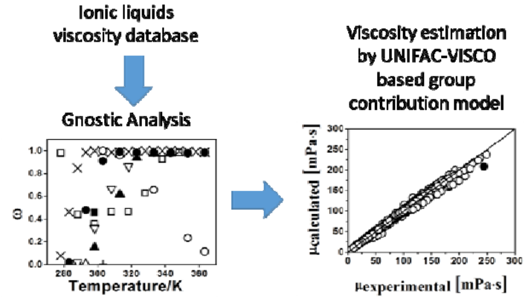


Figure 1: Methodology applied during this work.[2]

The estimation result showed a good agreement with experimental data with a relative absolute average deviation lower than 5 % in each case.[3] This novel approach will be presented and discussed in detail during this presentation.

Keywords: Electrolytes, UNIFAC-VISCO, UNIFAC-CONDUCTIVITY, Transport Properties, Estimation, Temperature, Composition.

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Oral Presentations

INFULUNCE OF TEMPERATURE TO THE HYDROCRACKING PROCESS OF MAZOUT IN THE PRESENCE OF A MODIFICATED HALLOYSITE

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At the present stage, the main task of petroleum refining industry is to raise the depth of oil processing involving heavy oil residues into processing with a view to increase the motor fuels production. Hydrocracking is one of the most effective processes of destructive refining of heavy residual raw materials for increasing production of high-quality motor fuels.

The purpose of the work is to investigation the obtaining process of fuel components from low-pressure hydrocracking of the mazout obtained from Baku oils in the presence of modificated suspended halloysite with transition metals (Ni, Mo) for obtaining additional (extra) light oil products in order to deepen the oil refining.

As seen from the results of experiments the depth of mazout hydrocracking in the presence of modificated suspended halloysite largely depends on process temperature. The influence of temperature to the hydrocracking process of mazout had been investigated in the interval of 400-440 °C at the pressure of 1.0 MPa. The yield of light petroleum products increases from 27.4 to 71 % mass. by increase of temperature from 400 to 440°C (pressure 1.0 MPa). The yield of gas, gasoline, diesel fraction and coke increases from 3 to 10, from 4.6 to 20.7, from 22.8 to 43.3 % and from 1 to 5 mass accordingly by the increase of temperature from 400 to 430°C. The yield of residue decreases from 68.6to 21 % mass. With further rise of temperature to 440 °C the yield of light petroleum products decreases from 71 % to 64 % mass, the yield of gas rises from 4.8 to 10 % mass. As temperature increases the rate of the cracking reaction rises faster than the hydrogenation reaction.

A change in temperature significantly influence the hydrocarbon content of the obtained products. So, with rise of temperature from 420 to 430 °C (P = 1.0 MPa, 2.5 % cat.) aromatic hydrocarbons content in gasoline decreases from 6.32 to 4.16 %, with further rise of temperature to 440 °C their content increases to 7.0 %, i.e. the dehydrogenation process takes place. With rise of temperature from 400 to 430 °C the content of iso-paraffins in gasoline fraction increases from 41 and 44% . With rise of temperature from 400 to 430 °C amount of sulfur decrease from 0,06% to 0,0280%, iodine number from 5.2 to 0.98 g J_2/100 g. Amount of sulfur of diesel fraction decrease from 0,17 % to 0,13 %, iodine number from 9.5 to 6.0 g J_2/100 g.

The obtained gasolines are characterized by a fine chromacity, low content of aromatic and unsaturated hydrocarbons, 70-71 points MON in a pure form. Diesel fraction is also characterized by the low content of aromatic hydrocarbons, what defines its high cetane number of 49-50 points.

The analysis of the quality of gasoline and diesel fractions shows that after the additional light hydrotreatment the obtained products can be recommended as commodity fuels of high quality.

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A NOVEL APPLICATION OF SURFACE ENHANCED RAMAN SPECTROSCOPY: MEASUREMENTS OF HEROIN IN BODY FLUIDS

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Heroin is one of the most common drugs of abuse, over a hundred years. Each year, public faces with millions of heroin related incidents such as deaths, intoxications, violent crimes, and diseases. Therefore, biological fluids of individuals who involved in these incidents need to be analyzed in terms of heroin use. In daily practice of forensic and clinical toxicology, professionals successively utilize GC-MS, GC-MS/MS, HPLC, LC-MS, LC-MS/MS, Q-TOF for drug in detection in biological fluids. However, these methods are extremely time-consuming and expensive. Therefore, professionals seek for cheaper and faster detection tools. Studies dealing with illicit drug analyses using Raman spectroscopy and Surface Enhanced Raman Spectroscopy (SERS) come up with positive results for trace analysis of heroin. In this respect, Surface Enhanced Raman Spectroscopy (SERS) is a promising alternative tool for heroin detection in biological fluids. In this study, we aimed to detect and measure heroin levels in spiked human blood, urine and saliva using SERS.

SERS calibration curve for heroin measurement was obtained by analysis pure heroin solutions of different concentrations on gold surfaces. Human blood, urine and saliva samples obtained from a healthy adult were spiked with equal amount of heroin solution. 1 µL of each spiked sample were dropped on to Raman active gold surface. After an incubation period of ten minutes Raman spectra gathered by a Raman Spectroscope with 785 nm laser source. Major peaks of heroin were determined as 407, 478, 627, 913, 1094, 1119 and 1341 cm^{-1}, respectively. Gathered spectra of heroin have been compared with those given in related literature.

The present study reveals a novel application of SERS in measurement of heroin in biological fluids, and points out a potential cheaper and faster method for forensic and clinical toxicology.

Keywords: Forensic toxicology, drugs of abuse, SERS, heroin, biological fluids.

THE INFLUENCE OF TEMPERATURE ON THE THERMAL CONDUCTIVITY AND VISCOSITY OF MULTIWALL CARBON NANOTUBES BASED NANOLUBRICANTS

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The suspensions of MWCNTs/oil have drawn much attention recently due the oleophilic property and the re-dispersion ability of MWCNTs. Nevertheless, there are still many questions about the behavior and the stability of their thermal conductivity and the viscosity under the influence of temperature. The main purpose of this study is to utilize the well-known three-omega method and an accurate viscometer for accurately measuring and inspecting the thermal conductivity and viscosity of multiwall carbon nanotubes nanolubricants with respect to temperature. For that, pure multiwall carbon nanotubes, without any special treatment, were dispersed in six types of commercial oils at three different weight concentrations (0.05, 0.1 and 0.3 wt.%) by ultrasonication and without using any stabilization method. It was observed that the sonicated tubes are separated, saturated, lubricated, and surrounded by oil layers, which not only ease its motion within the lubrication oil, but also counter balanced the Van der Waals forces which give them stability and the ability of detaching by applying any slight force. However, with the increment of temperature, the surrounding oil layers starts to decay. This allows, as a result, the surfaces of the MWCNTs to attract each other and agglomerate again. Moreover, convection currents act as agitator which also increases the contacts between the MWCNTs at higher temperatures. Microscopic video is presented to clarify this behavior during heating. The high sensitivity of the three-omega lab-made setup allowed to see the reflection of this behavior on the thermal conductivities of the nanolubricants. The results show that the thermal conductivity peaks at specific temperature and then decay to the value of the base oil. Moreover, it was also observed that the dynamic viscosity of the nanolubricant decreases dramatically with the increase in temperature. This behavior is due to the decrease in viscosity of the base oil, which is a result of declining the intermolecular forces of the oil itself. Moreover, the agglomeration of the heated MWCNTs also played a supportive role in this decrement.

Keywords: Nanolubricant, multiwall carbon nanotubes, thermal conductivity, viscosity, engine oil

EFFECT OF 1-ETHYL-3-METHYLIMIDAZOLIUM TETRAFLUOROBORATE AND SODIUM CHLORIDE ON THE LIQUID-LIQUID EQUILIBRIA OF 5-HYDROXYMETHYLFURFURAL, METHYL ISOBUTYL KETONE, WATER

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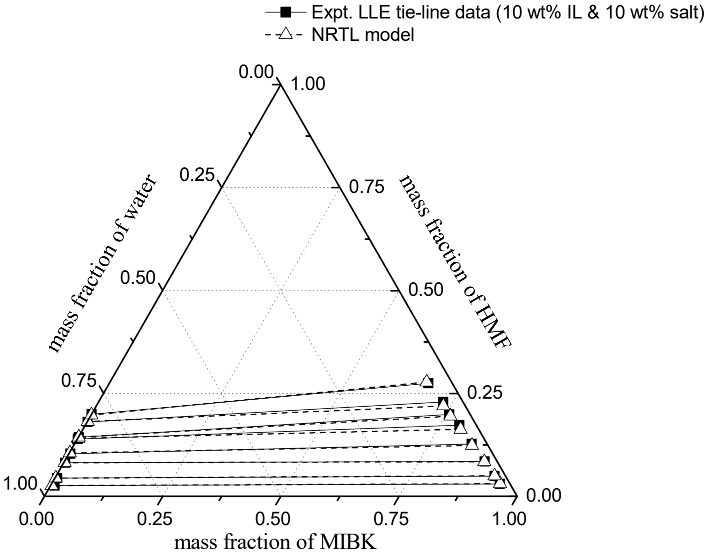
The use of bio renewable feedstocks seems to be particularly promising to overcome the dependence on fossil-fuel resources. HMF (5-hydroxymethylfurfural) is one of biobased platform chemical that can be converted to fuels and various chemical products. HMF is produced from a triple dehydration product of hexose which glucose and fructose are arranged as feedstocks. The production of HMF in aqueous-organic biphasic systems and ionic liquid solutions using organic solvent as an extraction solvent were selected as promising methods, since it can obtain high yield of HMF. Liquid-liquid extraction is one of the separation methods which is essential used in HMF production process to extract HMF more optimally. However, research on the systematic thermodynamics of HMF extraction is quite limited and needed to be developed. The objective of this study is to investigate the effect of ionic liquid [EMIM][BF_4] (1-ethyl-3-methylimidazolium tetrafluoroborate) and inorganic salt NaCl (sodium chloride) on the liquid-liquid equilibria (LLE) of HMF, methyl isobutyl ketone (MIBK), water systems at 313.15 K and atmospheric pressure. MIBK is chosen in this study as a potential extraction solvent for the separation of HMF. The separation factor (S) and distribution coefficient of HMF (D_2) were determined from LLE data to interpret the extraction performance. The results showed that the separation factor and distribution coefficient of HMF are lower in the presence of ionic liquid. However the addition of salt can enhance both these two key parameters making the extraction of HMF becomes favourable with S and D_2 values are higher than 1 for all range HMF compositions studied. The experimental LLE data were correlated well with the NRTL activity coefficient model. The RMSD (root mean square deviations) of the NRTL model were 0.93% for the HMF-MIBK-water-[EMIM][BF_4] and 0.32% for the HMF-MIBK-water-[EMIM][BF_4]-NaCl system. The NRTL binary interaction parameters of the investigated LLE systems were also generated in this study.

Keywords: Distribution coefficient, [EMIM][BF_4], 5-Hydroxymethylfurfural, Liquid-liquid equilibria, NaCl, Separation factor



Acknowledgement: This work was supported by LPDP (Indonesia Endowment Fund for Education), Ministry of Finance of the Republic of Indonesia, through Grant No. S-3937/LPDP.3/2016.

THERMODYNAMICS OF REDOX-ISOMERIC COMPLEXES WITH o-SEMIQUINONIC LIGANDS

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The redox-isomerism phenomena in solid state was discovered in o-semiquinonic complexes and attracts great attention because conversion of redox-states involves changes in magnetic properties as well as changes in the oxidation state and could find future application in memory devices and optical switches.

In adiabatic vacuum low-pressure and dynamic calorimeters the temperature dependence of the standart molar heat capacity of o-semiquinonic complexes with different neutral ligands and substituents in o-semiquinonic fragment has been determined at temperatures in the range T= (5 to 350) K mainly with an accuracy of about 0.2%. It was revealed that redox-isomeric transformation of semiquinon-catecholate form of studied complexes into bis-semiquinonic one accompanied by phase transition.
The enthalpy and entropy of the transformation were estimated and thermodynamic functions for the investigated complexes were calculated for temperature range T → 0 to T = 350 K.

In this work we have studied the influence of ligand nature and acceptor properties of substituents in o-semiquinonic fragment on thermodynamic parameters of phase transition related with redox-isomerism.

Acknowledgements: We are grateful to RFBR (grants №№ 16–03–00700a, 18-43-520030r_a) for financial support.

A NEW CODE FOR JOINT APPROXIMATION OF ENTHALPY INCREMENTS AND HEAT CAPACITY DATA

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Original experimental data on thermodynamic properties of substances in the condensed phase are often presented as tables and need to be approximated with functions that reproduce them with an acceptable accuracy. These functions can be used then for thermodynamic modeling and other theoretical studies. There are various codes for processing thermodynamic data. Some of them are meant for low-temperature heat capacity [I. Roslyakova, B. Sundman, H. Dette, et al // Calphad 55 (2016) 165], others for high temperature data measured by, for example, laser flash method. Moreover, there is a significant amount of methods for processing data on enthalpy increment obtained by classic calorimetry. Filling databases (IVTANTHERMO, NASA etc.) with new information on substances requires fitting data with preset polynomials [G.V. Belov, N.M. Aristova, I.V. Morozov, M.A. Sineva. // J. Math. Chem. 55 (2017) 1683].

A new computer program based on a combination of fitting algorithms is proposed for analyzing experimentally obtained enthalpy and heat capacity of substances in the condensed state. The program is supposed to unite all processing steps (low- and high- temperature heat capacity data, enthalpy increment data etc) to combine and analyze available data of several types simultaneously. The program has a friendly user interface. It comes in the forms of a standalone application and web application with limited functionality. The enthalpy increment data can be fitted by a polynomial of a chosen degree which can be used at the next step to process heat capacity dependence on temperature. Provided the user has high temperature heat capacity experimental data, it can be fitted by a polynomial combined of elementary functions picked manually or by preset combinations. The results can be exported in various database formats.

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NANOPARTICLE SYNTHESIS IN A MICROFLUIDIC CHANNEL

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Nano structures -with the increasing number of scientific research in the area- are capable of major changes in our life. However, the game-changing properties of nanostructures mostly are not repeatable. Moreover, it is not possible to produce the amount of nanoparticles necessary for the industrial world. Repeatable methods, which does not require highly trained personnel, for industrial scale production should be developed to transfer the academic research to the use of people.

For this purpose, various successful microfluidics device has been designed for microstructures synthesis. On the other hand, synthesis of nanostructure is not an enlightened area and there is a need for research to reach a better state. In this study, Many designs were made and best designs have been chosen with the light of the proper rheological values, microfluidics properties, and biopolymer's properties.

OPTIMIZATION OF A CASCADE COOLING CYCLE USING R236ea (1,1,1,2,3,3-hexafluoropropane) REFRIGERANT

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A variety of refrigerants are utilized in refrigeration systems. R236ea (1, 1, 1, 2, 3, 3-hexafluoropropane) has been proposed as an alternative for chlorofluorocarbons (CFCs) and hydro chlorofluorocarbons (HCFCs). HFC236ea has a zero ozone depletion potential (ODP) and low global warming potential (GWP). HFCF 236ea is used as a replacement for CFC114 for high temperature pump applications. HFC-236ea is used as a working fluid in Minichannel heat exchanger systems and low temperature organic Rankine cycles and also for low grade waste heat recovery. In this study, energy analysis of a cascade refrigeration cycle using R236ea refrigerant is performed. The thermodynamic properties of R236ea are calculated using Helmholtz equation of state. A simulation program in Java language has been developed for both calculate the thermodynamic properties for each region (liquid, saturated liquid-vapor mixture and superheated vapor) and analyze the refrigeration cycle. A program which was called "ref_cycle_opt. Java” was developed for optimization of a cascade refrigeration cycle that use R236ea as refrigerant, with use Graphic Search Optimization and Fibonacchi(Golden Search) Optimization methods. In this simulation study, energy analysis was performed by giving sample input values (evaporator heat flux 10 KW, evaporator saturated temperature 2^0C, evaporator pressure drop 5 kPa, evaporator superheated degree 2^0C, condenser saturated temperature 45^0C, condenser pressure drop 5 kPa, condenser cooling degree 2^0C, expansion valve enthalpy change 2 kJ/kg, compressor output temperature 100^0C and compressor mechanic efficiency 85%) for the refrigeration cycle. As a result, it has been observed that the system has achieved significant compliance with real refrigeration cycles.

EFFECTS OF DRYING TEMPERATURE ON THERMAL AND TEXTURAL PROPETIES OF PRECOOKED BUCKWHEAT GROATS

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Buckwheat is a pseudocereal belonging to the Polygonaceae family. It is used in food products due to its nutritionally valuable properties (rich in protein, lipid, dietary fiber and mineral contents) and it is a gluten free product. In this study, precooking process followed by drying was applied in order to obtain a new and nutritious ready to eat gluten free product as an alternative to bulgur (parboiled and dried wheat product). It was aimed to investigate dehydration behavior and rehydration characteristic of precooked buckwheat and to evaluate effects of processing on physical and thermal properties. Buckwheat groats were boiled for 30 minutes by using 3:1 buckwheat water ratio (w/w) then hot air drying was applied at three different temperatures. Experimental drying rate curves were obtained at 60, 70 and 80˚C at 1 m/s air velocity. The products obtained were analysed for water absorption capacity, color and Texture profile analysis (TPA) tests were applied using a texture analyser (Microstable Systems TA.XTExpress). Melting temperatures and enthalpies of the unprocessed, precooked and precooked dried and rehydrated samples were determined using Differential scanning calorimeter DSC (TA, Q2000 USA). Melting temperatures and enthalpies were found between 140-165˚C and 1100-1410 kJ/kg respectively.

VIBRATIONAL AND ELECTRONIC PROPERTIES OF $C_{16}H_{14}F_3NO_2$

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Photoactive organic dyes are very effective in light absorption and light electrical conversion in dye-sensitized solar cells and this directly affects battery efficiency. In today and in future studies, achieving optimum device efficiencies in dye-sensitized solar cells and extending the stable cell lifetime are priority issues to be addressed. Research and development studies on each of components dye-sensitized solar cells such as the electrode, electrolyte, semiconductor thin film and dye materials are continuing to improve battery efficiency [1].

In this study, it is aimed to theoretically and experimentally determine the structural, vibrational and some electronic properties of the coumarin based photoactive organic molecule used in the synthesis of dye-sensitized solar cells (DSSC). These properties of the title molecule were investigated by theoretical (DFT) and spectroscopic methods (FT-IR, UV-Vis and photoluminescence (PL) spectroscopy). In the DFT calculations, the B3LYP functional with 6-311G(d,p) basis sets were applied to carry out the quantum mechanical calculations. Excited state level (LUMO) of the molecule should be appropriately higher than the conduction band edge of used semiconductor. However, ground state level (HOMO) of the molecule has to be sufficiently lowers than the redox potential to regenerate the oxidized dye [2]. The plotted HOMO-LUMO and electronic structure data (E_{LUMO} and E_{HOMO} energy) of the coumarin based photoactive organic molecule were illustrated in Fig. 1. HOMO-LUMO energy gap (E_g) of $C_{16}H_{14}F_3NO_2$ molecule has been calculated 2.43 eV.

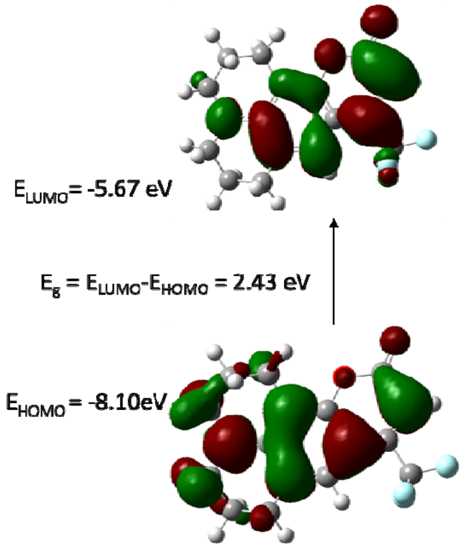

Fig.1. HOMO LUMO plot of the $C_{16}H_{14}F_3NO_2$ molecule by B3LYP/6-311G(d,p) level of theory

Keywords: Dye-sensitized solar cell (DSSC), Molecular modeling, Density Functional Theory (DFT), Coumarin.

Acknowledgments: This study was supported by Gazi University Scientific Research Projects Department (BAP project code: 05/2018-05).

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DEVELOPMENT OF THE IVTANTHERMO THERMODYNAMIC DATABASE FOR PURE SUBSTANCES

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Thermodynamic databases play essential role in a wide range of applications such as rocket engine engineering, nuclear power, chemical technology, metallurgy, resource usage, waste recycling, etc. The IVTANTHERMO information system [1] has made a significant contribution to the accumulation of thermodynamic data. It has been developed since 1966 in the Institute of High Temperatures of the Academy of Sciences of the USSR. Nowadays its development is continued in the Department for Thermophysical Data of JIHT RAS.

The IVTANTHERMO system includes the database which contains more than 3400 substances, formed of 96 chemical elements, as well as supplementary software for analysis of experimental results, data fitting, calculation and estimation of thermodynamical functions an thermochemistry quantities. In this report we present the next version called "IVTANTHERMO-Online" [2]. It has a new extensible database design, user-friendly web interface with client-server architecture and a number of features for online and offline data processing. The new system enables to handle multiple versions of each block of data, to store additional information for users and experts (such as comments, bibliography, experimental data, molecular structure, etc.), to present data in multiple forms, to attach calculation services and link with other databases. The substances can be searched using their names, formula, atomic composition or CAS numbers. The supplemented software includes modules for calculation of chemical composition and data fitting.

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MEASUREMENT OF LIQUID POLYMER COMPOSITE WITH ATO PARTICLES BY PULSE AND STEP-WISE TRANSIENT TECHNIQUES

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The measurement of the thermal properties of liquids using the heat source covers the problems of heat flow by convection that disturbs the regular temperature response. To avoid convective part of the heat transport mechanism, the experimental conditions should be arranged in a special way. The turbulent and laminar flow of the liquid appears at the higher values of generated heat flux density. So the very low power is allowed to use. The liquid flow creates streams of the heated matter. The heat transport of the liquid via these streams is faster than the conductive part of the heat flow. Due to the statistical principle of this effect, we can found the fluctuation of the temperature in radial direction across the sample cross section as well as in time when we measure the temperature in one point. As the consequence the statistical increases and decreases in the temperature response are present.

The paper discusses the measurement regime and related experimental arrangement to avoid the disturbance effect caused by convective mechanism of the heat flow.

The polymer composite sample was measured in a liquid state and antimony tin oxide (ATO) particles were diluted in a form of typical colloid dispersion. Experiment was done in a special chamber that was developed for the measurement of the materials with non-solid consistence. The analysis of the heating regime in relation with the recording time of the temperature response show the limits in the power used for generation of the temperature response. The problem in pulse transient technique is that the heat that invokes measurable height of the temperature response is generated in relatively short time. So the step-wise regime is more advantageous as the total heat should be generated in longer time and with much lower heat flow density.

The paper discusses also the results obtained by transient techniques that use pulse and step-wise form of the heat generation. These results indicate that high values of the specific heat of the nanocomposite polymer with ATO particles predict its use for the heat-blocking properties. Thus it is suitable as the thermal barrier in the thermal management applications. More often it is deposited on window glass of buildings to improve the energetic efficiency of the buildings and lower the heat losses.

Acknowledgement: This work was supported by the Slovak Academy of Sciences under the contract No. 2/0192/17 ”Development of sensors and measurement methods for transient techniques for the measurement of thermophysical properties of materials and their application for seasonal storage of heat energy” in cooperation with COLVER, s.r.o. company, that provided the composite material.

THERMOPHYSICAL PROPERTIES OF THE (CO_2 + N_2) SYSTEM FROM ACCURATE INTERMOLECULAR POTENTIAL ENERGY SURFACES

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A new CO_2–N_2 intermolecular potential energy surface has been developed based on highly accurate quantum-chemical *ab initio* computations of pair interaction energies. An analytical representation of the pair potential has been used to determine the CO_2–N_2 cross second virial coefficient and values for the traditional transport properties in the dilute gas limit for the (CO_2 + N_2) system at temperatures up to 2000 K.

The cross second virial coefficient was calculated using the Mayer-sampling Monte Carlo method of Singh and Kofke [1]. Quantum effects were accounted for by using an effective pair potential following the approach of Feynman and Hibbs [2].

Values for the thermal conductivity, shear viscosity and the product of density and self-diffusion coefficient in the zero-density limit have been calculated with the TRAJECT program [3] utilising the new pair potential in conjunction with previously published pair potentials for the two pure substances [4, 5]. We present the new potential energy surface and a comparison of our results for the calculated values of the thermophysical properties with the best available data from the literature.

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DEVELOPING OF A REAL TIME REFRIGERATION CYCLE SIMULATION

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In this study, a real time refrigeration simulation program is developed. A refrigeration cycle is based on four different equipment: an evaporator, a condenser, a compressor and an expansion valve. Evaporator is modelled by using boiling heat transfer , one phase heat transfer (heat is taken from the evaporator by water stream) as finite element model. Similarly, condenser is modelled by using condensation heat transfer and one phase heat transfer as finite difference model. Compressor and expansion valve are also modelled seperately. Thermodynamic properties of refrigerants are modelled as equation of state, furthermore thermophysical properties of refrigerant and secondary fluid(water) such as viscosity, thermal conductivity, surface tension are also modelled. All these modelled are combined as a real time refrigeration cycle which can be received input variables from some outside program or datalogger or control cards such as PLC , Arduino or rasbery PI. Simulation systems are prepared in java programming environment which can be used as real time programming and serial channel communication environment. The basic aim of such systems is to train artificial intelligence systems for refrigerant system control.
Keywords: Real time refrigeration cycle, real time programming, simulation

EXPERIMENTAL DETERMINATION OF DIFFUSION COEFFICIENTS OF CARBON DIOXIDE IN ETHYL ACETATE AND N-BUTANOL

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Global warming is one of the most important challenges of today’s world and the primary reason of this climate change is accepted as the increment of carbon dioxide (CO_2) concentration, one of the greenhouse gases that has a great impact on air pollution, in the atmosphere. There are some conventional systems used in order to decrease the emission of CO_2 from the major point sources, flue gases; but these systems require so much energy in absorption and regeneration units. Thus, investigation of alternative solutions is currently an important global research topic.

In this study, CO_2 absorption into ethyl acetate and n-butanol is investigated. Both of these chemicals are environmentally friendly and are relatively cheaper to produce. These make them great alternative to conventionally used chemicals like amine solutions. Since there is not enough information about them in literature, experimental studies have been carried out to determine the diffusion coefficient of pure CO_2 in pure ethyl acetate and n-butanol. The CO_2:N_2O analogy method was considered and the experiments were carried out using a diaphragm cell at 293 K and 90.8 kPa atmospheric pressure. By a pressure transmitter, the decrement in pressure due to absorption and diffusion of CO_2 in solutions was monitored and recorded. Diffusion coefficients were calculated by these pressure drop data.

Firstly, the characterization of diaphragm cell was done with a known binary system in which the diffusion of N_2O in water was performed and the diaphragm constant was calculated as $\xi = 7836\ m^{-1}$. As the second step, experiments were done for the diffusion of N_2O in ethyl acetate and CO_2 in water and in ethyl acetate. The diffusion coefficient N_2O in ethyl acetate was found as $1.867 \cdot 10^{-9}\ m^2.s^{-1}$ and those for CO_2 in water in ethyl acetate were calculated as $1.514 \cdot 10^{-9}$ and $1.984 \cdot 10^{-9}\ m^2.s^{-1}$, respectively. The analogic ratio constants of N_2O and CO_2 gases in water and ethyl acetate are very close to each other and the experimental results are in good agreement with literature. Thus, these showed that the experimental system was reliable and can be used for other solvents.

Third step of the experiments were then performed with CO_2 and n-butanol. Since N_2O is reactive with alcohol, the analogy method utilizing N_2O in n-butanol for the diffusion coefficient calculation for this specific system could not be used. So, for n-butanol, the experiments were performed directly with CO_2. The diffusion coefficient was calculated as $1.325 \cdot 10^{-9}\ m^2.s^{-1}$.

With this work, the diffusion coefficients of CO_2 in ethyl acetate and n-butanol which can be alternative solutions to commercial and conventional CO_2 capturing solutions are obtained at the specified operating conditions. The high boiling points (BP) of the selected absorption solutions lead to low solution losses due to evaporation in the industrial operations. For this reason, the ethyl acetate (BP = 350 K) studied in this work may be a good alternative to commercially used methanol (BP= 338 K). Similarly, n-butanol (BP = 391 K) has also the potential to be an alternative to the amine solutions commonly used in the industry (monoethanol amine (BP = 443 K) and diethanol amine (BP = 544 K)) because it reduces high energy requirements during the solvent recovery step in the process.

Keywords: Diffusion coefficient, carbon dioxide, absorption, ethyl acetate, n-butanol.

INITIAL VALUE ESTIMATION FOR NON-LINEAR ROOT FINDING OF EQUATION OF STATES SOLUTIONS

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Equation of states are usually given in the form of pressure, $P(T,v)$, or Helmholts equation, $A(T,v)$ form. Most of the time, independent properties of the given equation is temperature and specific volume(or density). Thermodynamic space is non-continious due to phase change and critical point occurance and properties (specially specific volume-density) has differs thousand times in different region. For most root finding methods, if first initial estimation is too far out it may not give a solution, therefore first initial value estimation for a given set of known thermodynamic pair is an important part of EOS computer programming and simulations. Given thermodynamic data should always check again critical point and saturation point values to get some idea about which region solution should be fallen. Furthermore, utilisation of cubic EOS such as Suave, Peng-Robinson etc will give us additional approximation. Due to nature of cubic EOS equations, by using cubic equivalent and solving it analitically by using historical Tartaglia-Cardano (ca.1500) formula $v(T,P)$ values can be obtained. Even though cubic equation of states are not as accurate as modern EOS's. The value obtained form cubic roots will serve as a good initial estimation by combining the knowledge from saturation and critical point data. It should be not that in order to use cubic EOS in general means, critical temperature, critical pressure and Pitzer acentric factor should be known. Pitzer acentric factor is defined for reduced temperature $T_r = T/T_c$. $T_r = 0.7$ as a function of reduced vapor pressure $P_{vpr}(T_r)$ by the following formula: $\omega = -\log\left[P_{vapor}(T_r = 0.7)\right] - 1.0$

Keywords: Thermodynamics, Cubic equation of states, Root finding, initial value estimation

MULTIDIMENSIONAL OPTIMISATION FOR A REFRIGERATION CYCLE FOR VARIOUS OPERATION CONDITIONS

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Selection of correct refrigerant and best possible operation parameters to obtain maximum possible COP in a refrigeration cycle is quite important. In this study, a wide spectrum of equation of states are developed to model thermodynamic and thermophysical properties of refrigerants, then by using these equation of states a refrigeration cycle model that can be operates for all these refrigerants are developed. Cycles optimise to find the maximum COP for different refrigerants and different operation conditions and for each operation condition order of refrigerants that given the best COP is found. As Optimisation process several stochastic optimisation methos used to avoid possible errors. And so the best refrigerants and best possible operation conditions obtained for each different cases that investigated. The actual example cases given in this paper, is for the purpose of the sampling the possiblity of optimisation. Due wide variety of parameters, the tool will be more valuable to avaluate the actual cases and situations that existed in the objective cycles and operating conditions.

Keywords: Thermodynamics, refrigeration cycle, stochastic optimisation, refrigerant selection.

THERMAL DIFFUSIVITY OF POLYMER BASED NANOCOMPOSITES WITH GRAPHENE NANOPLATES: THE SIZE EFFECT

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High density polyethylene (HDPE) is the one of most widely used thermoplastic due to its regular chain structure, perfect mechanical properties, high melting temperature, good electrical insulation and due to the combination of energy demand and low cost for processing [1]. Despite its remarkable properties, the low thermal conductivity of HDPE limits its application areas. Thus, many studies have been focused on enhancing the thermal properties of HDPE. One common way to solve this problem is to add conductive filler materials into HDPE. Among conductive filler materials, graphene has attracted considerable interest in recent years due to its unique 2D structure and superior properties, such as high electron mobility, high thermal and electrical conductivity and good mechanical properties [2].

This study aims to investigate the effect of different dimensions (diameter (D) and thickness (t)) and contents (1 to 10 vol %) of graphene nanoplates (GNPs) on the thermal diffusivity of HDPE nanocomposites. GNPs have been used as received, without any purification treatment: iGP (t=50-100 nm, D=~44 µm), iGP2 (t=5-8 nm, D=~5 µm) and iGP3 (t=50-100 nm, D=~5 µm). All samples have been prepared by melt mixing method, followed by compression molding. Thermal diffusivity measurements have been carried out by modulated photothermal radiometry. The thermal diffusivity of nanocomposites increases with increasing GNPs loading in all cases. It is found that iGP having the largest diameter provides higher enhancement in thermal diffusivity than the others. GNPs with the same diameter, irrespective of their thickness, exhibit approximately the same thermal diffusivity values.

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MIXING ENTHALPY FOR BINARY MIXTURES CONTAINING IONIC LIQUIDS

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Ionic liquids (ILs) are very attractive materials as they could be used different applications dealing with chemistry, chemical engineering, energy, gas storage and separation or materials science. To design proper chemical engineering processes using these relatively novel materials, the prior knowledge of their energetics of mixing is crucial, particularly, to establish the energy and environmental cost of possible applications. Furthermore, this allows to gain a better understanding of the interactions between these fluids and the different substrates in solution to design proper ILs to be used in a given process. However, due to the relative novelty of the field, the published datasets are sometimes controversial. [1] This fact can be attributed to different reasons: (i) difficulties in controlling the purity and stability of the ILs; (ii) availability of accurate experimental techniques, appropriate for the measurement of viscous, charged, complex fluids; and (iii) choice of an appropriate clear thermodynamic formalism to be used by an interdisciplinary scientific community. During this talk, all these points will be discussed as well as the way to treat the information obtained by an appropriate thermodynamic formalism in order to show progress to be made in this field.

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EFFECT OF PHASE CHANGE MATERIALS ON THERMAL AND MECHANICAL PROPERTIES OF POLYPROPYLENE

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Phase change materials have received great interest in many applications especially as thermal energy storage materials. PCMs due to their high latent heat of fusion are capable of storing or releasing large amounts of energy by melting and solidifying at certain temperatures. Different inorganic and organic substances were already utilized for the creation of phase change materials. In this study paraffin wax based phase change materials, being chemically inert, stable and commercially available at relatively low cost, were mixed into polypropylene at 20, 30, and 40 wt% by twin screw extruder. After obtaining of PCM filled polypropylene granules with strand pelletizer, composite plates were fabricated by injection molding. The effect of PCMs on the mechanical and thermal properties of PP composites was investigated by tensile tests, melt flow index, thermal gravimetric analysis and differential scanning calorimetry.

Keywords: polypropylene composites, phase change materials, mechanical properties, thermal properties.

CARBON DIOXIDE SOLUBILITY IN 1-ETHYL-3-METHYLIMIDAZOLIUM TRIFLUOROMETHANESULFONATE

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Due to some unique and benign solvent characteristics, ionic liquids (ILs) have established themselves in multiple technical applications. The rather low-priced ionic liquid 1-ethyl-3-methylimidazolium trifluoromethanesulfonate (or triflate) [EMIM][TFO] is hydrophilic, and displays particularly good thermal and electrochemical stability [1]. Additionally, there is plenty of consolidated thermophysical data available for [EMIM][TFO] [2].

In this presentation, we report about experiments to determine the high-pressure solubility of carbon dioxide in [EMIM][TFO] at temperatures T = (273.15 to 413.15) K and pressures p up to about 5 MPa, which are performed by a so-called pressure-drop isochoric method at preset temperatures. The apparatus and the operational procedures of the solubility measurements are described in detail in our previous papers [3,4]. The solubility is measured in a stainless-steel equilibrium cell that is placed inside a thermostat. The temperature in the measuring cell is controlled by a thermostat with an uncertainty of $\Delta T = \pm$ (30 to 100) mK using a (ITS-90) PT100 thermometer. The temperature directly in the measuring cell is monitored by another PT100 thermometer. A pressure transducer indicates the pressure of CO_2 filled to the gas reservoir, which is measured with an experimental uncertainty of Δp = 0.1 %. Temperature inside the gas reservoir is also controlled and it was measured using the PT100 thermometer with an experimental uncertainty of $\Delta T = \pm$ 45 mK. The solubility measurements were carried out in decrements of ΔT = 20 K within the investigated temperature range and at four different determined pressure steps. The first pressure is the maximum possible pressure (i.e. about 5 MPa) created in the gas reservoir. The other steps with maximum pressure are: second step – about 3 MPa, third step – about 1.5 MPa, and the final step – about 0.5 MPa.

Within the p,T-range investigated, CO_2 displayed a solubility in [EMIM][TFO] from a mole fraction x = 0.0274 and a corresponding molality m = 0.1083 mol·kg^{-1} at T = 413.15 K and p = 0.415 MPa up to x = 0.5021 and m = 3.8749 mol·kg^{-1} at T = 293.15 K and p = 3.995 MPa. The estimated total uncertainty of CO_2 solubility in the IL using this method is approximately $\Delta x = \pm$ 0.00005 mole fraction or $\Delta m = \pm$ 0.0001 mol·kg^{-1}. The measured solubilities as a function of temperature and pressure were fitted to a virial equation using either the mole fraction x or molality m of the ionic liquid. The solubility of CO_2 in [EMIM][TFO] monotonously decreases with increasing temperature or, in other words, at a fixed pressure less gas is dissolved in the IL when the temperature becomes higher. The temperature dependency of Henry’s law constant was calculated from the solubility data. Thermodynamic properties (such as the Gibbs energy of solvation $\Delta_{sol}G$, enthalpy of solvation $\Delta_{sol}H$, entropy of solvation $\Delta_{sol}S$, and heat capacity of solvation $\Delta_{sol}c_p$) of solution were calculated at various temperatures T from the correlation of Henry’s constant by applying the well-known thermodynamic relations of solution to evaluate the solute–solvent molecular interactions.

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A PRELIMINARY STUDY FOR OPTIMIZED HEAT EXCHANGERS: PARAMETRIC ANALYSIS OF AXISYMMETRIC CIRCULAR GROOVED MODEL

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It has been shown that grooved pipes are thermally more efficient than the smooth pipes. Compared to rectangular, trapezoidal and other groove geometries, the circular ones are proved to be the most efficient in terms of heat transfer. Different than the previous studies in which the groove dimensions are constant along the pipe, we study the effect of groove radius and the gap between adjacent grooves on the local heat transfer coefficients using computational fluid dynamics (CFD) software (ANSYS Fluent). The computational domain presented in Figure 1 has a long smooth inlet section (L=10D) that provides the flow with being fully developed. The grooved section consists of three sub-sections to see the effects of groove dimension in stream-wise flow direction. Each section includes five grooves with constant radius in each one. We vary the radius of circular grooves parametrically in each section to optimize the local groove radius throughout the pipe.

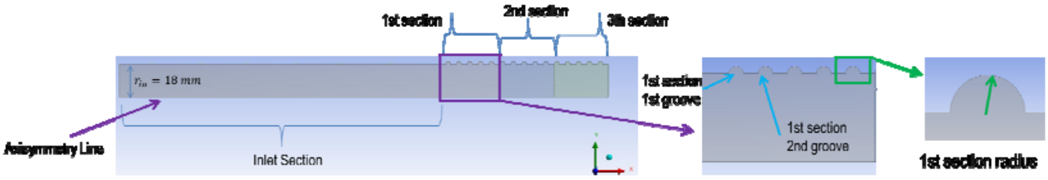

Figure 1. The circular grooved axisymmetric model.

We couple the fluid flow (Re=2304) with energy equations, and the grooved sections are set as heated wall at constant temperature of 350 K. The optimal mesh has been selected by performing mesh independence study and finer mesh has been used in heated wall section. The radii of grooves are varied from 6 to 8 mm with an increment of 0.2 mm considering the manufacturability of the pipe, to do so we use the design of experiments (DOE). After DOE process, local heat transfer coefficient values of all groove parts are examined in response surface module. We observe that the relation between local heat transfer coefficient and groove radius is nonlinear. Maximum local heat transfer coefficient values are obtained at not only extreme design points but also at intermediate points (Table 1). Figure 2 shows the variation of local HTC of the first and last sections, respectively, as a function of other sections' groove radii.

Table 1. Maximum and minimum heat transfer coefficient (HTC) values.

		1st groove radius (mm)	2nd groove radius (mm)	3th groove radius (mm)	HTC (W/m^2.K)
1st part	Min.	6.4	6	6.8	**8.3626**
	Max.	6	8	6.6	**8.6038**
2nd part	Min.	6.6	6	6	**5.8374**
	Max.	8	8	6.4	**6.0793**
3nd part	Min.	8	6	6.4	**5.0267**
	Max.	6	8	6.6	**5.3455**

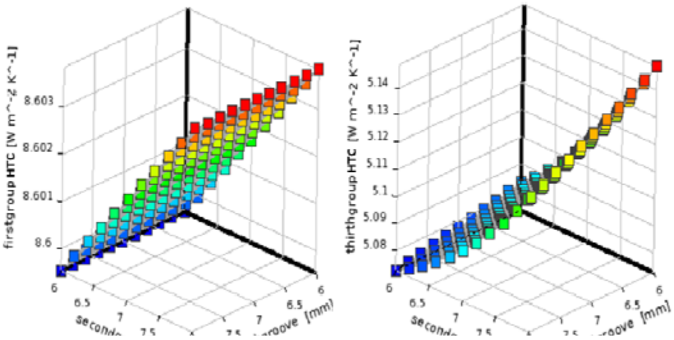

Figure 2. Backward and forward effect on HTC.

We show that, for the first section, the maximum HTC is achieved when the groove radius is maximum in the second section; the third section has almost no effect. For the third section, however, the maximum HTC is achieved when the radius of first section is minimum and radius of second section is maximum. It can be deduced that different groove radii throughout the model can be used to improve the local heat transfer coefficient and grooved models with constant groove dimensions are inadequate for thermal optimization.

THERMAL CHARACTERIZATION OF A HEAT EXCHANGER OPTIMIZED FOR ADDITIVE MANUFACTURING

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Associated with the development of 3D printer technology, heat exchangers can be manufactured by additive manufacturing besides the traditional production methods. The design freedom introduced by additive manufacturing also reveals the idea of implementing the topology optimization approach into HVAC (Heating, Ventilation and Air Condition) systems. In this study, an optimized air-to-air heat exchanger model was additively manufactured and experimentally examined (Fig. 1) in terms of thermal efficiency.

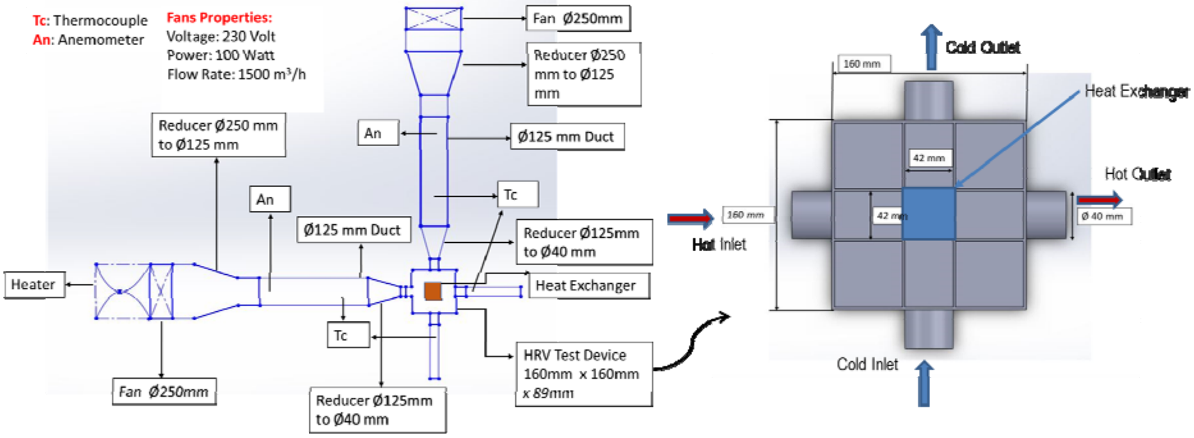

Figure 1. Experimental setup.

The heat transfer surface geometry ıf the cross-flow heat exchanger model is obtained from a recently published topology optimization study and this design is additively manufactured with different thermoplastics (ABS, HIPS, PA-CX12). A rectangular finned heat transfer surface that has same hydraulic diameter with the optimized model is selected as the base design and also additively manufactured. The experimental results are compared by means of thermal efficiency which is calculated at different air flow rates. The results show that the optimized heat exchanger model for all thermoplastic materials is thermally more efficient than base model (Fig. 2). In addition to that ABS is the most effective thermoplastic material due to its high thermal conductivity.

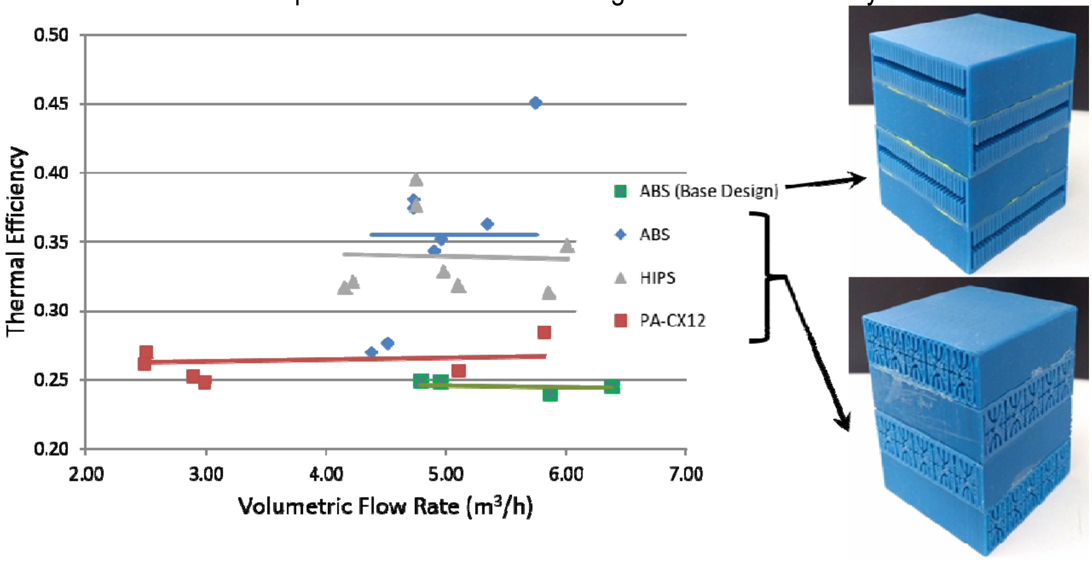

Figure 2. Experimental results for different heat exchanger material and models.

NEW FORMULATION FOR THE VISCOSITY OF ISOBUTANE

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Thermophysical property data of high standard are urgently requested for industrially important fluids to design more accurately compressors, gas turbines, and gas pipelines as well as cooling cycles and chemical processes. Transport properties, generally and particularly in the region near the critical point, are not known with sufficient accuracy, if compared with thermodynamic properties. For isobutane, the current NIST standard data base REFPROP 9.1 of Lemmon et al. (2013) recommends the viscosity correlation of Vogel et al. (2000) characterized by uncertainties of (3-4)% in its range of validity. This correlation was predicated on an outdated equation of state (EoS) of Younglove and Ely (1987), whereas REFPROP 9.1 recommends the reference EoS of Bücker and Wagner (2006) for the thermodynamic properties of isobutane.

In 2015, a vibrating-wire viscometer combined with a single-sinker densimeter was applied by Herrmann et al. to perform very accurate viscosity measurements on isobutane, including the near-critical region. The standard uncertainty of the data was conservatively estimated to be 0.3% so that they could be considered as primary data.

The contradiction between the new reference EoS and the outdated EoS and the improved data situation in the dense-gas region prompted us to generate a new viscosity formulation for isobutane using a state-of-the-art structure-optimisation method. The concept of the new formulation incorporates four contributions concerning the limit of zero density, the initial-density dependence, the near-critical and the higher-density regions. The first two contributions were separately treated, in which the second benefitted from the kinetic theory. Whereas the critical-enhancement contribution was partly pre-treated, the thermodynamic scaling approach was used for the very high-density region. Computed values for the new formulation were compared with the primary data sets employed when generating the formulation, but also with values calculated for the previous viscosity correlation of Vogel et al. (2000).

DETERMINATION OF RADIONUCLIDES ALONG TRANSBOUNDARY RIVERS OF AZERBAIJAN

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Azerbaijan is a country of small rivers. There are more than 8550 rivers in its area. Only 21 of them have 100 km long in the country area. All rivers in the end flow to Caspian Sea, some of these directly flow into Caspian Sea, others by Kura and Araks rivers. It is well known that 80% of Azerbaijan territory lies within of is affected by the Kura–Araks watershed. In the meantime Kura and Araks rivers and its tributaries are natural drainage system for 100% of Armenian storm and sewage waters and 52% of Georgian waters. Mean 30×10^9 m^3 waters which formed in Turkey, Georgia, Armenia, Iran and Azerbaijan goes to Caspian Sea annually. Most of these waters are considered as surface water and are using intensively both for agricultural, municipal and industrial usage. Azerbaijan uses Kura water also for drinking which makes river water quality items very sensitive to the needs of the community.

The present study was conducted to investigate radionuclide contents in water, soil and sediment samples, which were collected from 19 different points along rivers Kura and Araks during 2017 year. Samples were delivered after homogenization and storage for1 month for equilibrium (in Marinelly beakers) and gamma-spectrometry analyses (Ge – high resolution gamma spectrometer).

In the investigated water samples only K^{40} isotopes were observed, which change in range 1.04-3.3 Bq/l. Natural radionuclides as Ra226, Ra228, K40 and artificial radionuclide Cs137 concentrations were evaluated for both bottom sediment and soil samples. The concentrations of the analyzed radionuclides in sediment samples were as following: Ra226 ranged between 11.91-25.68 Bq/kg, Ra228 ranged between 16.07-36.39 Bq/kg, K40 ranged between 249.6-625.1 Bq/kg, and Cs137 ranged between 0.42-3.39 Bq/kg,activity of Co60 and Cs134 were below MDA (minimal detectable activity). Maximum activity for noted radionuclides was observed in bottom sediment samples taken from Arpachay, near of Armenian boundary. The concentrations of the analyzed radionuclides in soil samples were as following: Ra226 ranged between 10.96-19.35 Bq/kg, Ra228 ranged between 15.68-25.88 Bq/kg, K40 ranged between 322-582.6 Bq/kg, and Cs137 ranged between 0.54-7.55 Bq/kg,activity of Co60 and Cs134 were below MDA. The dependence of radioactivity from the water parameters was determined for the sediment samples. It was obtained that, change in water quality as a result of natural, anthropogenic effects and seasonal changes can increase the accumulation process of the radionuclides in bottom sediments.

THERMOPYHYSICAL PROPERTIES OF BINARY 1-BUTYL-3-METHYLIMIDAZOLIUM TRIS(PENTAFLUOROETHYL)TRIFLUOROPHOSPHATE + METHANOL MIXTURES

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Ionic liquids and their organic mixtures are interesting to be useful as heat transfer fluids in absorption refrigerating and solar heating systems. Such application of substances requires high quality thermophysical properties. In this work, we present the new density measurements of 1-butyl-3-methylimidazolium tris(pentafluoroethyl)trifluorophosphate [BMIM][FAP] and methanol binary mixtures at the wide range of temperature [T=(273.15 to 413.15) K] and ambient pressures with an estimated experimental relative combined standard uncertainty up to $\Delta\rho/\rho$= ±0.03 % in density, which were investigated using a Anton-Paar DMA HPM vibration-tube densimeter. Measurements were made for 12 concentrations from x=(0 to 1) mole fraction of methanol (x=0.0, 0.1220, 0.2182, 0.4964, 0.7462, 0.8876, 0.9391, 0.9650, 0.9806, 0.9920, 0.9979, 0.9994 and 1.0).

The density values $\rho(p_0,T)$/kg·m^{-3} at ambient pressure and at temperatures T = (273.15 to 413.15) K were investigated using the combination of the Anton Paar DMA 5000M, DSA 5000M and DMA HPM vibration tube densimeters with an uncertainty of $\Delta\rho$ = ± (5·10^{-3} to 3·10^{-1}) kg·m^{-3}. The speed of sound values $u(p_0,T)$/m·s^{-1} at ambient pressure and temperatures at T = (283.15 to 343.15) K are investigated using the Anton Paar DSA 5000M vibration tube densimeter and sound velocity meter with intervals of ΔT= (5-10) K and an uncertainty of Δu= ± 0.1 m·s^{-1}.

An empiric equation for fitting of the density values of [BMIM][FAP] and methanol mixtures has been developed as a function of pressure, temperature and mole fraction of methanol. The excess molar volumes V_m^E /cm^3·mol^{-1} and apparent molar volume V_ϕ /cm^3·mol^{-1} of the investigated mixtures were calculated using the pure components and mixture properties.

Keywords: Ionic liquid, density, excess molar volume, apparent molar volume, thermophysical properties.

COMPRESSIBILITY OF HYDROCARBON FLUIDS AFTER INJECTION WITH CO_2 AND THE EFFECT ON THE MECHANICAL PROPERTIES OF PETROLEUM ROCK FORMATION

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The mechanical properties of a rock formation significantly depend on the properties and saturation of the fluids occupying the pore space in rock frame, as well as the mineral matrix of the rock. Although fluid mechanical properties of reservoir fluids are systematic and primarily depend on fluid density, however, under different environment, such as when supercritical CO_2 is injected in the geological formation, the fluid phase and its mechanical and thermodynamic properties can vary dramatically. Injection of CO_2 at elevated temperature and pressure can result in density crossover due to dramatic increase in the density of supercritical CO_2. For example, when pressure increases from 20 to 80 MPa at 400 K, density of decane only increases by 6% (from 665 to 720 kg/m^3) but for CO_2 considerably increases by 60 % (from 350 to 857 kg/m^3) crossing over the hydrocarbon phase density, while bulk modulus of decane remains four times higher (1.14 GPa) than that of CO_2 (0.25 GPa). In this work, we report isothermal compressibility and isobaric expansivity of a mixture of supercritical CO_2 + decane ($C_{10}H_{22}$) at temperatures up to 410 K and pressures up to about 80 MPa, for CO_2 mole fractions from (0 to 0.87). An equation of state for compressed liquid density has been optimized to reproduce the experimental data measured in this work and all other data reported in literature for this system, with an average deviation of $\pm 0.002\rho$. The effect of CO_2 injection on mechanical properties of rock formation (rarely studied) is also demonstrated using the Gassmann model as a function of CO_2 concentration at different pore pressures and porosity. Accurate data on these mechanical properties are required for reliable design of well-completion and minimizing risk in drilling operations.

GLOBAL ISOMORPHISM BETWEEN MOLECULAR FLUIDS AND ISING-LIKE MODELS

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Zeno-line and asymmetry effects of liquid-vapor equilibrium for molecular fluids are considered within the global isomorphism with the Ising-like models. The latter is based on the geometric reformulation of the (approximate) linearities of the density binodal diameter (the rectilinear diameter law) and the unit compressibility line (the Zeno-line). The correspondence takes the form of projective mapping between thermodynamic states of a fluid and the Ising model. We demonstrate how the parameters of the transformation depend on the interaction potential in cases of Lennard-Jones and Yukawa fluids. We discuss explicit relations between the bulk thermodynamic functions as well as surface tension of molecular fluids and the Lattice Gas (Ising) model in 2D and 3D cases. On this basis we derive the relation beyween the critical compressibility factors of molecular fluids and the lattice gas [1]. We show how the associative properties of a fluid can be taken into account via the structure of the isomorphic lattice. Surface tension can be considered similarly on the basis of the known results on the Ising model [3,4]. Recent results have been obtained within the Fulbright Research project 2017-2018 (IIE ID: PS00245791).

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APPLICATION OF THERMO- AND FLUIDDYNAMIC MODELS FOR SIMULATION OF INTERACTION IN HUMAN-CLOTH-ENVIRONMENT SYSTEM

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The paper presents study of coupled aerodynamic and thermodynamic interaction between human body and environment under low temperature and wind conditions. The body generates the heat within certain organs which is then transferred by the thermal diffusion through the body substance possessing very non uniform properties. A large fraction of the heat generated by internal organs is transported to the body periphery by a complicated net of blood vessels. The heat penetrates through the cloth and is then transferred to surrounding medium by natural and forced convections. We used two models simulating the inner human body thermodynamics: the model of Fila and the model based on the heat flux selected using experimental data. In the second case the inner body thermodynamics is not resolved. The heat flux is selected from the condition that the surface temperatures take experimental values for certain environmental condition.

Wind causes big areas of the overpressure on the cloth surface which results in deformations and local change of the cloth thickness. In its turn, change of the local thickness leads to an alteration of heat conduction properties of the cloth. This means that the heat exchange between body and air is changed not only by intensification of convective heat transfer but also due to change of thermodynamic properties of cloth caused by wind induced deformations. The second effect which has still not been discussed thoroughly in the literature is in focus of the present paper. Under strong wind conditions the heat transfer from the human body can sufficiently be increased due to change of the thermal conductivity caused by cloth deformation under wind induced pressures. For instance, at 10 m/s the heat increase could be of ten percent.

To keep the human body temperature on the acceptable level, the local heating elements can be embedded into the cloth textile. The power of this heating was calculated using the models of aero-thermodynamic coupled interaction including heat radiation. The results of the work are used for the design of real protection cloth for the work under low temperatures and wind conditions in oil gas industry.

CURRENT POSSIBILITIES OF FUEL AND LUBE OIL INVESTIGATION AND DEVELOPMENT OF NEW METHODS

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The Laboratory for fuels and lubricants is specialized for determination of fuel and lubricant parameters as well as pollutants in various environmental matrices. The well-equipped laboratory offers options e.g. for determination of boiling characteristics of fuels, rheological investigations of non-Newtonian fluids, surface tension and ash forming components in fuels. In addition to analytics according to current specifications, we offer the development and validation of new analytical methods for fuels and lubricants.

We implement investigations into efficiency tests of newly developed fuel and lubricant additives, the examination and quality assurance of new test fuels as well as to contribute to their standardization. Furthermore, we adapt or new develop suitable analysis methods for the characterization and monitoring of system solutions developed at our institute for technical machines and plants.

Selected methods for the determination of thermodynamic properties of fuels and lubricants as well as examples for new developed methods will be presented.

SYNTHESIS OF NEW MACROHETEROCYCLES AS CONVENIENT CHELATORS FOR DRUG DELIVERY SYSTEMS

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Macrocyclic compounds are an important class of compounds that serve as ligands, catalysts, sensors, drugs, organic semiconductors, liquid crystals and materials for nonlinear optics. One of the widespread application area is using them as a drug delivery systems. Historically, there were two sources of macrocycles for drug delivery: natural products and peptides. However, more synthetic macrocycles have been developed and studied in recent years.

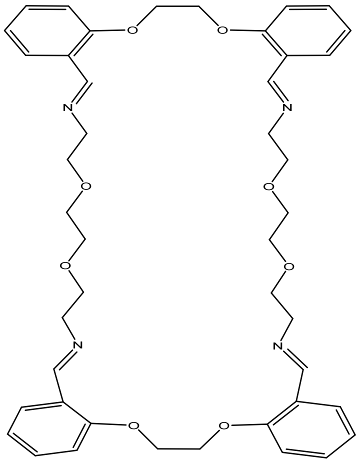
Macrocycles are preferred for drug delivery for the following reasons:

1. Their strict conformations limit the products produced and the ability to react, so there are reduced side effects.
2. Macrocycles have reduced flexibility.
3. Macrocycles have reduced polarity which increases the cell permeability of the resulting molecule. More polar side chains result in more active transport across a cell membrane will more nonpolar side chains passively permeate the cell. Intramolecular hydrogen bonds are also credited with a modest increase in cell permeability.

These characteristics make macrocycles ideal as enzyme inhibitors, G protein-coupled receptors (GPCRs) and protein-protein interaction inhibitors.

Taking into account all these advantages, we synthesised forty and forty two membered new macroheterocycles (I and II) on the basis of dialdehydes, which were obtained on the basis of salicylaldehyde. The reason of using of salicylaldehyde as a basis for dialdehydes is caused by the fact that the proton in hydroxyl group is acid and in the alkaline medium can be easily replaced resulting in obtaining of dialdehyde. Another point is that obtained macroheterocycle at the end will have at least two oxygen atoms in the cycle.

As it can be seen from the structure, both macroheterocycles contain 12 heteroatoms in cycle. In addition to this, second one contains hydroxyl group, which can play an important role in the formation of hydrogen bond and enhance its chances to be used in drug delivery systems.



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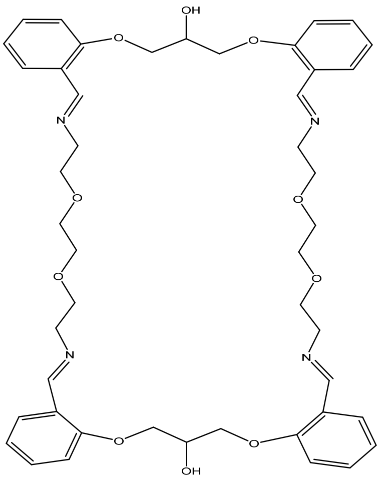

II

THERMODYNAMIC PROPERTIES OF DIATOMIC ARGON COMPOUNDS

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The diatomic argon compounds are of importance for different plasma sources that contain argon as a basic gas. One of these applications is the mass spectrometry with inductively coupled plasma (ICP-MS). In such experiments the signals from the argon compounds can disturb measured spectra significantly. Therefore, for accurate processing of the ICP-MS results it is necessary to obtain the thermodynamic functions of the compounds of argon with other gases (H, O, etc.) and metal ions. It allows to estimate concentrations of these compounds in the ICP-MS plasma.

In this work we report on thermodynamic properties of the following substances: ArV+, ArCo+, ArAr, ArAr+, ArH and ArH+. As a starting point, we use DFT and quantum-chemistry data to find an appropriate model for the interatomic interaction potential. Then the rovibronic spectra is obtained via numerical solution of the Schrödinger equation for each electronic state that contribute to the total internal partition function. The thermodynamic properties are calculated from the partition function within the ideal gas approximation. This method differs from the typical approach based on the use of molecular constants. The influence of various interatomic potential models on the final results is discussed.

FIRST-PRINCIPLES STUDY OF DEFECTS IN CdMn(Fe)Te. EFFECT OF γ-IRRADIATION ON OPTICAL PROPERTIES OF CdMn(Fe)Te EPITAXIAL FILMS

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Ab initio calculations were used for electronic structure of the ideal and defective semiconductors Cd1-xMn(Fe)xTe (x=0.01-0.25). It was defined band gap, density of states, total energy, magnetic moments, number of electrons, Fermi levels, defect formation energies and threshold energies. It is determined that the band gap in Cd1-xMn(Fe)xTe increases linearly with an increase in the Mn (Fe) concentration, but there occurs an insignificant decrease in the lattice parameter with Mn(Fe) concentration increasing. It is determined that defects lead to an increase in the band gap width, formation of additional magnetic moments, local levels in the forbidden band, and also to a change in the type of conductivity which are confirmed experimentally.

$Cd_{1-x}Mn(Fe)_xTe$ epitaxial films were obtained on glass substrates in a vacuum (1-2)10^{-4} Pa by the Molecular Beams Condensation method. It is determined the optimal conditions for creation of epitaxial films with perfect structure and clean, smooth surface, by using of additional source of Te vapor.

Absorption and transmission spectra of $Cd_{1-x}Mn_xTe$ (x=0.07) epitaxial films on glass substrates of thickness d=15μm and 22μm have been studied. The band gap width of $Cd_{1-x}Mn_xTe$ (x=0.07) epitaxial films was Eg=1.62eV. The studies of the effect of γ-radiation on the optical properties of epitaxial films showed that there occurs a change in the band gap width, absorption and reflection coefficients, which can be explained by the appearance of the local levels from the formation of defects. Results corresponds to our theoretical calculations.
This work was supported by the Science and Technology Center in Ukraine, Grant № 6150 and № 6288.

MOLECULAR INSIGHT INTO THERMODYNAMICS OF THE LIQUID ISOPROPANOL+WATER MIXTURE

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There is significant interest in aqueous alcoholic mixtures e.g. due their importance for numerous technical applications, like electron transfer reactions, heterogeneous catalysts or fuel cell technology. Their high complexity in terms of physico-chemical properties also makes their study attractive for the development of theoretical approaches. Molecular modeling and simulation has become a powerful route for interpreting experimental data on thermodynamic properties, but it critically depends on the force field that describes the molecular interactions. In this work, a new force field for isopropanol is presented. It is based on quantum mechanical data and it allows to accurately predict the time-dependent and time-independent physico-chemical properties of this secondary alcohol.

Having validated the performance of the force field for the pure alcohol, a wide range of properties of the binary mixture 2-propan-ol + water are predicted with different molecular simulation techniques in the entire composition range. These results are interpreted from a molecular point of view. The predictions reproduce experimental transport coefficient data of the binary liquid mixture at 298.15 K and 0.1 MPa and are in good agreement with the excess volume and enthalpy. The association pattern, which can convincingly be sampled by molecular simulation, offers an explanation to the physico-chemical behavior of this aqueous alcoholic mixture.

ISOLATION AND CHARACTERIZATION OF OKRA POLYMERS

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Okra plant fruits Abelmoschus esculentus (family - Malvaceae) is one of the most popular vegetable which is cultivated in tropical, subtropical, and warm temperate regions worldwide. Okra pods contain mucilage which is known as rich sources of polysaccharides such as D-galactose, L-rhamnose, and L-galacturonic acid and gives its slimy viscous characteristic. This mucilage has a good potential for pharmaceutical and food industries as thickeners, emulsion stabilizers, suspending agents etc. but the functionality of plant-resourced biopolymers are highly effect from their physicochemical properties. Therefore, in this study the okra polymer was extracted from okra pods and pyhsical, chemical, thermal and rheological properties of the okra polymer were examined. Also, the surface morphology of the okra polymer was analyzed by scanning electron microscope (SEM).

The polymer was extracted from dried and milled okra pods and after extraction process, samples were dried by freeze drier and milled (<260 μm). The physical and chemical properties of the samples were determined by bulk density, compressive density, Hausner index, compressibility index, loss of drying, solubility, rheological measurements, pH and swelling. The flow properties of the polymer solutions which prepared at different concentrations were determined at 25 °C using a TA DHR 3 Rheometer. TA Instrument (TA Q2000) was used to study the thermal characteristics of the okra gum. About 5mg sample was placed in an aluminium hermetic pan and was scanned at -10 ºC to 220 ºC at a scanning rate of 5.00 ºC/min. Nitrogen was used as purged gas at a flow rate of 50 mL/min.

The moisture value of okra polymer was found to be 11.452±0.042%. The compressibility index, the bulk density, the compressive density and the Hausner ratio were found 25.926±1.777, 0.269±0.005, 0.365±0.01 and 1.35±0.032, respectively. Solubility and swelling index of the polymer were determined 31.839±5.85% and of 3.335±0.175%.

Flow behavior characteristics of the solutions at different concentrations (1, 2, 3, 4 w/v) of the samples were examined. It was determined that the viscosities of the solutions increased as the concentration of the polymer solution increased. Power Law, Herschel Bulkley and Bingham models were tried to determine the flow characteristics and it was determined that the model that best represents the flow behavior for all samples is the Power Law model. Based on the analysis conducted using DSC, the glass transition temperature (T_g) and melting point (T_m) of okra gum are 47.57±0.24ºC and 164±4.58ºC, respectively.

In this study, physical, chemical, thermal and rheological properties of the okra polymers were determined. Extraction and characterization of the okra polymers have been carried in order to find new applications in the medical, pharmaceutical and food industries.

COMPARATIVE INVESTIGATION OF MECHANICAL PROPERTIES OF JUTE AND FLAX FABRIC REINFORCED COMPOSITES

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Mechanical properties of epoxy based hybrid composites reinforced with jute and flax woven fabric were investigated comparatively to analyze the performance difference due to the stacking sequence of two different natural bast fibres.

For this purpose, two different composite plates with symmetrical and non-symmetrical sequences, consisting of four layers of jute and four layers of flax fabric were produced by vacuum infusion method. For increasing the amount of adhesion between reinforcement and the matrix, alkali treatment was applied onto the reinforcement fabrics separately prior to composite manufacture. Impact tests at three different energy levels and tensile tests were performed. Force-deflection and energy-time graphs were established with the data obtained. Impact damage images were analyzed.

Test results showed that the mechanical properties of hybrid composites were affected by stacking sequence of fabrics. The stacking of fabrics in symmetric sequence has resulted in higher tensile strength. On the other hand, impact test results showed that the composite with non-symmetrical sequence had a better impact performance. Furthermore, in the non-symmetric sequence, when the impact load is applied to the jute side, it is found that this type of composite absorbs more impact energy and that less damage occurs on the lower surface.

As a conclusion, it can be recommended that is if the hybrid composite is to be subject to tensile loads symmetric sequence would be advisable, but in the case of impact loading to choose jute fabric reinforcement in the upper layers having non-symmetric sequence is advised.

Acknowledgement
This study was supported by the "115M168" project number and the "3001-Initial R & D Projects" Support Program by TÜBİTAK.

AMIDOXIMATED POLY[*N*-(3,4-DICYANOPHENYL) ACRILAMIDE]: SYNTHESIS, CHARACTERIZATION AND THORIUM SORPTION PROPERTIES

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Removal of long-lived radionuclides from nuclear waste solution is an important aspect in nuclear waste management. Thorium is a long-lived naturally occurring radionuclide widely distributed over the earth crust. Thorium also originates both from the nuclear industry and from other anthropogenic activities When radionuclides are released into the environment, they eventually reach the top of the food chain to be ingested by humans and other animals, causing several health problems [1]. A number of techniques including chemical precipitation, ion exchange, reverse osmosis and adsorption have been developed to recover thorium from aqueous solutions. At low concentrations, separation through adsorption of long-lived radionuclides such as thorium from aqueous solution is important in nuclear/radiation chemistry and environmental/waste treatment chemistry [2].

Polymers with specific functionalities can be obtained by either synthesizing new monomers carrying the functional groups capable of interacting with the target metal ions followed by polymerization by converting groups on existing polymers or copolymers with suitable reactants into the desired functional groups. It has been determined that the polymers containing amidoxime groups have a tendency to form complexes with heavy metal ions, the complex with thorium ions being one of the most widely investigated [3].

The aims of this study are to synthesize a new monomer carrying two adjacent pendant nitrile groups, preparation of its polymer and finally conversion of the reactant nitrile groups into amidoximes, and to investigate the influence of various experimental parameters on Th adsorption by synthesized polymer.

4-aminophthalonitrile and acryloyl chloride were used to synthesize the *N*-(3,4-dicyanophenyl) acrilamide monomer and this monomer was polymerized to poly[*N*-(3,4-dicyanophenyl) acrilamide]. Finally, polymer was converted into the amidoximated form containing nitrile groups. The structure of monomer, polymer and its amidoximated form were characterized by FT-IR spectroscopy and thermal analysis methods. The influence of various experimental parameters such as contact time, pH, initial concentration, and temperature on Th(IV) adsorption by amidoximated polymer was investigated and conditions for the adsorption of thorium from aqueous solution were determined. Adsorption of Th(IV) onto amidoximated polymer has been evaluated in terms of equilibrium, kinetics and thermodynamics studies. The isotherm models, such as Freundlich, Langmuir, Temkin and Dubinin-Radushkevich have been used to describe the equilibrium data. Kinetic data obtained from the batch adsorption studies were fitted to pseudo-first order and pseudo-second order equations. Th(IV) adsorption by amidoximated polymer was pH dependent (pH range, 4.5–7.5) and maximum sorption was observed at pH 7.0. Adsorption process is well described by Langmuir isotherm in comparison with Freundlich, Dubinin–Radushkevich (D-R) and Temkin isotherms. Thermodynamic data ($\Delta H°$, $\Delta S°$, $\Delta G°$) were calculated from the temperature dependent sorption isotherms. $\Delta H°$ and $\Delta G°$ values are obtained as 72.48 J/mol and -6.12 kJ/mol at 298 K, respectively. Results suggested that the adsorption of Th(IV) on amidoximated polymer was a spontaneous and endothermic process. According to comparison of kinetic models applied to the adsorption of Th(IV) onto amidoximated polymer, the experimental data fitted very well the pseudo-second order kinetic model.

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QUASI-STATIC BENDING BEHAVIOR OF SANDWICH STRUCTURES WITH BALSA CORE

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This study investigates the three-point bending behavior of balsa wood-based bio-sandwich structures with thermoplastic skins. Additionally, failure mechanism of the structures are also evaluated within the research. Balsa wood (BALTEK® SB 100) with thickness of 15 mm and E-glass reinforced polypropylene-based prepregs are used as the core and face sheet materials, respectively. Hot-press method is utilized for the fabrication of sandwich structures. The typical thickness of the sandwich panel is obtained as 16.55 mm. Afterwards, the structure is cut into specimens with 150 mm length and 25 mm width. Flexural tests are performed according to the standard (ASTM C 393-00) using a Shimadzu AG-X (100 kN) Universal Testing Machine with a crosshead speed of 2 mm/min and a span of 100 mm. The tests are maintained until the samples lose their load-carrying capacity. Herewith, the load-displacement responses of the specimens are reported. Within the study, four flexural tests are performed for inference. The figure exhibits a sandwich specimen mounted on the three-point bending test setup. The experimental results indicate that the maximum loads vary between 710 N and 822 N. As to the failure mechanism, the main failure mode seems to be debonding between the face sheets and core material.

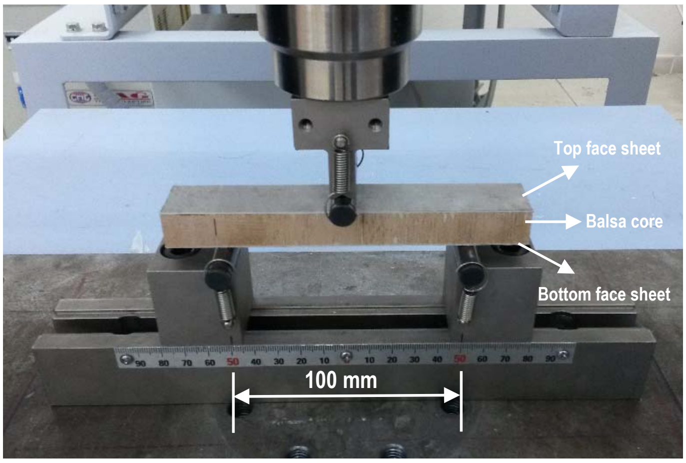

Figure: Photograph of the three-point bending test set-up

UNDERSTANDING NONIDEAL MIXING OF PROTIC IONIC LIQUIDS: MD SIMULATIONS AND LATTICE MODELS

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We report results of molecular dynamics (MD) simulations characterizing the hydrogen-bonding in mixtures of two different protic ionic liquids sharing the same cation:Triethylammonium-Methylsulfonate (TEAMS) and Triethylammonium-Triflate (TEATF). The Triethylammonium-cation acts as a hydrogen-bond donor, being able to donate a single hydrogen bond. Both, the Methylsulfonate- and the Triflate-anions can act as hydrogen-bond acceptors, which can accept multiple hydrogen bonds via their respective SO_3-groups. In addition, replacing a Methyl-group in the Methylsulfonate by a Trifluoromethyl-group in the Triflate significantly weakens the strength of a hydrogen bond from an adjacent Triethylammonium cation to the oxygen-site in the SO_3-group of the anion. Our MD simulations indicate that these subtle differences in hydrogen-bond strength significantly affect the formation of differently sized hydrogen-bonded aggregates in these mixtures as a function of the mixture-composition. Moreover, the reported hydrogen-bonded cluster sizes can be predicted and explained by a simple combinatorial lattice model, based on the approximate coordination number of the ions, and using statistical weights that mostly account for the fact that each anion can only accept three hydrogen bonds. Based on the simple lattice model, we introduce a lattice mixture model for mixtures of protic ionic liquids, including the effect of hydrogen bonding redistribution. We show the observed non-ideal negative mixing energies as a function of the mixture composition can be solely explained by hydrogen-bond redistribution.

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A NEW ABSOLUTE METHOD FOR THE ENTHALPY OF FUSION MEASUREMENTS UP TO 1000 °C WITH AN UNCERTAINTY BETTER THAN 0.3 %

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The French National Metrology Institute (*Laboratoire National de Metrologie et d’Essais*) has developed a new calibration and measurement procedure in order to enhance the uncertainty of its measurements of enthalpy of fusion from 23 °C to 1000 °C. This new measurement procedure consists in putting the studied sample inside a calibration crucible and in performing the heat calibration of the calorimeter by electrical substitution (Joule effect) at two temperatures before and after the temperature of fusion of the sample during the same low-rate heating run. When the fusion of the sample is detected, an electrical compensation of the fusion is launched. The quantification of the electrical energy necessary to melt the sample, which can be measured with high accuracy, and the integrated remaining heat flow rate divided by the calibration factor (sensitivity) of the calorimeter at the temperature of fusion, lead to the determination of the enthalpy of fusion of the sample with low uncertainty.

In addition to the fact that this procedure directly takes into account the temperature dependence of the sensitivity and keeps the calibration and measurement experimental conditions strictly the same, it reduces the influence of the uncertainty component associated with the area of the peak of fusion when no electrical compensation is applied. Uncertainties of the enthalpy of fusion measurements, performed by using this facility and this new procedure, have been assessed according to the “Guide to the Expression of Uncertainty in Measurement” (GUM). The relative expanded uncertainty (k=2) associated with the enthalpy of fusion measurement is better than 0.2 % for tin and indium and is about 0.3 % in the case of silver. These uncertainties are promising for the certification of reference materials as energy standards for differential scanning calorimeters.

Keywords: Enthalpy of fusion, calibration, electrical compensation, uncertainty

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BIOSYNTHESIS OF SILVER NANOPARTICLES USING PROPOLIS EXTRACT AND EVALUATION OF THEIR ANTIBACTERIAL ACTIVITY WITH SPECTROSCOPIC METHODS

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This study aims to investigate anti-bacterial potential of silver nanoparticles (Ag-NPs) synthesized by a green chemical procedure using propolis extract as a capping agent. The successful formation of Ag-NPs was confirmed by ultraviolet-visible (UV–vis) spectrometer, transmission electron microscopy (TEM) and Fourier transform infrared spectroscopy (FTIR). TEM study showed that the formed Ag-NPs were spherical in shape with an average particle size of ~15 nm. Furthermore, the Ag-NPs exhibited good antibacterial activity against *Bacillus thuringiensis* and *Staphylococcus aureus* (Gram-positive bacteria), *Escherichia coli*, and *Pseudomonas aeruginosa* (Gram-negative bacteria). Among the bacteria tested, *Pseudomonas aeruginosa* was found to be most susceptible to the Ag-NPs.

Keywords: Biosynthesis, propolis, silver nanoparticles, antibacterial potential

SIMULATIONS ON THE STRUCTURE, VIBRATIONAL AND ELECTRONIC PROPERTIES OF METHYL -2-CHLORO-6-METHYLPRIDINE-4-CARBOXLATE BY FT-IR, FT-RAMAN AND DFT METHODS

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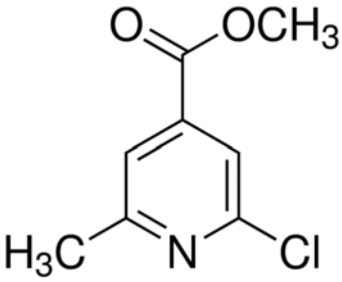
To the best of our knowledge DFT calculations and experimental studies on infrared spectra of Methyl -2-chloro-6-methylpridine-4-carboxlate have not been reported so far. Therefore, we have carried out detailed theoretical and experimental investigation on the vibrational spectra of this compound completely.



Molecular structure

The calculations were performed at DFT levels by using Gaussian 09 [1-2] program package, invoking gradient geometry optimization [3-4]. The optimized structural parameters were used in the vibrational frequency calculations at the DFT level to characterize all stationary points as minima. Then, vibrationally averaged nuclear positions of title compund were used for harmonic vibrational frequency calculations resulting in IR and Raman frequencies. In the present work, the DFT method B3LYP with 6-311G(d,p) basis set were used for the computation of molecular structure, vibrational frequencies and energies of optimized structures. The vibrational modes were assigned on the basis of TED analysis for 6-311G(d,p) basis set, using SQM program [5].

Keywords: Methyl -2-chloro-6-methylpridine-4-carboxlate, Molecular modeling, Density Functional Theory (DFT)

Acknowledgments: This study was supported by Gazi University Scientific Research Projects Department (BAP project code: 05/2018-06).

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ULTRAFAST RELAXATION IN MICELLAR SURFACTANT SOLUTIONS: IS THIS STAGE OBLIGATORY?

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Self-aggregation in surfactant solutions reveals as spontaneous formation of a number of micelles as stable surfactant aggregates at surfactant concentrations above the critical micelle concentration. In the course of time, the aggregation equilibrium is established in a micellar solution and the concentrations of aggregates containing different numbers of surfactant monomers become fixed. Relaxation to the aggregation equilibrium in a micellar solution occurs gradually. The stages of fast and slow relaxation are usually distinguished in this process [1,2]. Ultrafast relaxation of premicellar aggregates with small aggregation numbers has been reported in some works devoted to the numerical study of the time evolution of micellar systems [3-5]. The aim of this communication is to show that ultrafast relaxation is an inevitable stage of micellar relaxation at any initial conditions and to describe the spectrum of the characteristic times of ultrafast relaxation both numerically and analytically [6]. This is performed by analyzing the spectrum of the eigenvalues of the matrix of kinetic coefficients of the linearized Becker−Döring equations for aggregate concentrations. The matrix of kinetic coefficients is determined by the minimal work of aggregation and by the diffusivities of surfactant monomers and aggregates. From that point it is a subject of statistical thermodynamics. The first value of the spectrum ordered as an ascending series is equal to zero, thereby corresponding to the law of conservation of the surfactant. The second value is very small; it differs from the series of subsequent values by several orders of magnitude and determines the time of slow relaxation. The other eigenvalues describe the processes of fast relaxation and comprise the contributions from the relaxation processes in both micellar and premicellar regions of aggregate sizes. Here the contribution of the ultrafast relaxation can be numerically distinguished. The obtained result is confirmed by the analysis of the spectrum of relaxation times of premicellar aggregates as a closed system. The spectrum of ultrafast relaxation times is mainly determined by the first diagonal elements of the matrix of the linearized Becker–Döring equations and can be described analytically.

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Keywords: statistical thermodynamics, nanofluids, micelle, kinetics, relaxation, aggregation

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THERMAL CONDUCTIVITY OF NANOMATERIAL

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There is considerable interest in understanding heat transport in nanomaterials [1, 2]. Nanomaterials 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 nanomaterials 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. A theory of the thermal conductivity has been developed for nanomaterials made by embedding nanoparticles in a host dielectric material. The phonon dispersion relation has been calculated using the transfer matrix method in the long-range approximation, where the phonon wavelength is larger than the size of the nanoparticle. We found that these nanomaterials have two phonon branches known as ω_k^+-phonon and ω_k^--phonon branches. For both phonon branches, the density of states and the phonon velocity are calculated. The thermal conductivity is evaluated with the Kubo formalism and the Green's function method for both ω_k^+-phonon and ω_k^--phonon branches. It is also found that the density of states, phonon velocity and thermal conductivity for both phonon branches depends on the size of the nanoparticle, spacing between nanoparticles, and the phonon refractive index of the nanoparticle and the host material. In the long wave approximation, expressions of the phonon conductivity, the density of states and the phonon velocity have very simple forms which can be used by experimentalists to explain their experiments or plan new experiments. We have also applied our theory to explain the experimental thermal conductivity data of silica-resin, alumina-resin, AlN-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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P-V-T PROPERTIES AND VISCOSITIES OF BINARY SYSTEMS CONTAINING OLIGOMERIC POLYETHYLENE GLYCOL AND THE IONIC LIQUIDS WITH DIISOPROPYLETHYLAMMONIUM CATION

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The protic ionic liquids (PILs) and polyethylene glycol (PEG) are considered as highly potential absorbents for capturing carbon dioxide. The solubility of carbon dioxide in the blends of these two compounds could also be substantially high. Since the *P-V-T* properties and the viscosity data of the absorbents are crucially important for developing the process technology of carbon dioxide capture with absorption-desorption operations. The densities (ρ) were measured for the binary mixtures containing oligomeric PEG (PEG-200, its average molecular weight about 200 g/mol) with the new protic ionic liquids (PILs), diisopropylethylammonium propanoate [DIPEA][C_2COO] and diisopropylethylammonium octanoate [DIPEA][C_7COO] at temperatures from 298.2 K to 348.2 K and pressures up to 50 MPa over entire composition range. Additionally, the viscosities (η) of the same ionic liquid-PEG systems were also measured at atmospheric pressure. The excess molar volumes (V^E) were calculated from the density data and then correlated with a modified Redlich-Kister model. While S-shape variations of isothermal-isobaric V^E with composition are found from the [DIPEA][C_2COO]-containing system, negative values of V^E over the whole composition range are found from [DIPEA][C_7COO]- containing system. Moreover, the deviation of mixture’s viscosity from a mole fraction average ($\delta\eta$) was also calculated from the experimental results. Those values are positive over the entire composition range and are also well correlated with a Redlich-Kister-type model. The density data of pure components and their mixtures obtained from this study were correlated satisfactorily with the Flory-Orwoll-Vrij (FOV) and the Schotte equations of state, respectively. The characteristic parameters (P^*, V^*, and T^*) for each component were determined from the density data of the pure fluid and the binary interaction parameter (Δ_{12}) was determined from the density data of each binary system.

MEASUREMENTS OF THE DENSITY AND VISCOSITY OF GEOTHERMAL FLUIDS FROM DAGESTAN (SOUTH RUSSIA) GEOTHERMAL FIELD

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Geothermal fluids plays a significant role in nature as geothermal systems. The thermodynamic data on geothermal brines, which can be considered as mixtures of aqueous solutions of NaCl, KCl, $CaCl_2$, $MgCl_2$, *etc.*, are needed for geothermal thermal energy utilization devices. The underground water (geothermal fluids) are the largest reservoir of aqueous electrolyte solutions. The volumetric (density and derived properties such as partial and apparent molar volumes), caloric (heat capacity and enthalpy), and transport properties (viscosity and thermal conductivity) data of the geothermal fluids are important in geothermal exploration and energy production, for example, to establish optimal operations for the productions of geothermal brine fields. Also accurate thermophysical properties data of the geothermal brines are prerequisite for chemical and reservoir modeling of geothermal brine systems (multi-phase underground flows) and fundamental importance for the understanding of various physic-chemical processes occurring in the natural environment (quantify the natural processes occurring below the surface). To understand and control those processes which used geothermal fluids, it is necessary to know their thermodynamic and transport properties, particularly density and viscosity as a function of temperature. The energy properties of the geothermal fluids may be extracted directly from the *PVTx* properties of the geothermal fluid through standards thermodynamic approaches. If the *PVTx* properties of the geothermal fluid are known, the energy properties may be readily calculated. The available *PVTx* properties of geothermal fluids are not sufficient to meet the needs of the geothermal industry for complex solutions such as those found in geothermal reservoirs. Prediction flow parameters for a production well is of central interest for the use of geothermal energy.

Thermophysical properties of geothermal fluids such as density, viscosity, heat capacity, and enthalpy play a fundamental role in mass and heat transfer in the Earth’s interior. In order to provide numerical modelling of the heat and mass flow processes of geothermal fluids using concentration equations, definitions of the thermodynamic properties of density (ρ), viscosity (η), and enthalpy (h) of these fluids are required. Solution of the set of differential equations (equations of mass conservation, linear momentum, and energy conservation) for mathematical simulations of the Earth’s interior considerable depend on thermodynamic properties of geothermal brines (density, enthalpy, and viscosity) as a function of temperature, pressure, and concentration of salt (minerals). Solving these sets of equations enables the determination of such quantities as T and P gradients at a point in the flow, and T, P, x profile in time and space.

Density and viscosity of natural geothermal fluids from the Kayakent wells (No. 4 and No. 5) of Dagestan Geothermal Field (South Russia) have been measured over the temperature range from (278 to 333) K and at atmospheric pressure. The measurements were made using the Anton Paar DMA4500 densimeter and Stabinger SVM3000 viscometer. The measurements were made for two geothermal fluid samples from the hot-wells (No.4 and No.5) of south Russia (Dagestan, Caspian seashore). The combined expanded uncertainty of the density, viscosity, and temperature measurements at the 95 % confidence level with a coverage factor of $k = 2$ is estimated to be 0.0005 % (for DMA4500) and 0.02 % (for SVM3000), 0.10 %, and 0.01 K (DMA4500) and 0.005 K (SVM3000), respectively. Measured values of viscosity were used to develop theoretically based Arrhenius-Andrade type viscosity model, which reproduced the measured values of viscosity within 0.9 % to 1.7 %. The measured densities and viscosities were compared with the values for geothermal brine models (binary and ternary aqueous salt solutions, synthetic brines).

Keywords: geothermal fluids, density, vibrating tube densimeter, viscosity, water

Poster Presentations

SOME OF THE THERMODYNAMIC FUNCTIONS OF INCR$_2$TE$_4$ COMPOUND

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Some thermodynamic parameters of the triple InCr$_2$Te$_4$ compound have been calculated for the first time. Primarily, the atomization energy of InCr$_2$Te$_4$ was calculated taking into account the energy of atomization of compound components [1]. It was calculated, that $H_S(InCr_2Te_4)$=45,73 kcal/mol. Then calculations of the heat capacity and standard entropy of the compound were performed [2]. The calculation of the heat capacity is also possible by the Debary method [3]. Based on calculated values of the $\theta'_D / 298$ function, the isochoric thermal capacity of components was computed and by summing up them according to Nyman-Kopp rule the isochoric heat capacity of the InCr$_2$Te$_4$ was calculated. We calculated the isochoric heat capacity of the InCr$_2$Te$_4$ also by Magnus-Lindeman equation [4]:

$$C^o_{p298} = C^o_{v298} + 1{,}45m\left(\frac{298}{T_{mel.}}\right)^{\frac{3}{2}}. \tag{1}$$

The standard entropy of the compound relative to the heat capacity can be calculated by Hers equation (method) [3]:

$$S^o_{298} = K_r\left(M / C_{p298}\right)^{\frac{1}{3}} \cdot m \tag{2}$$

where K$_r$ – a fixed number that takes quantities from 2.5 to 8.5, depending on the degree of ionization of the chemical bonding, M – the molar mass of the compound. For chalcogenides K$_r$=4 cal/mol·K. Taking these into account, the equation (2) can be written as follows:

$$S^o_{298} = 28\left(M / C_{p298}\right)^{\frac{1}{3}}. \tag{3}$$

In Kelly method, by giving a certain value of the entropy to each ion, the entropy of a compound can be finding by summing the entropies of separate ions: It should be noted, that for the calculation of thermodynamic functions of InCr$_2$Te$_4$, the primary data included in formulas (1)-(3) are taken from [1]. From our calculations C_{V298}=37,84 cal/mol·K. The average values of isochoric heat capacity and standard entropy computed by different formulas are $C_{p298}(\text{average price}) = 38{,}74\frac{cal}{mol \cdot K}$ and $S^o_{298}(\text{middle}) = 72{,}93\frac{cal}{mol \cdot K}$.

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LIQUID PHASE OXIDATION OF NAPHTHENE-PARAFFINIC HYDROCARBONS OF DIESEL FRACTION IN THE CATALYTIC PRESENCE OF REDUCED GRAPHENE OXIDE

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Perspectivity of hydrocarbons aerobic liquid-phase oxidation processes is determined by saving of the synthesis products with high selectivity, significancy and easier handling, comparatively [1]. Experimental use of liquid-phase oxidation reactions by air oxygen of hydrocarbons, separated from oil or oil fractions in the presence of special catalysts, activating both O_2 molecule and oxidation substratum, leads the reaction for forming of target product. A wide range of acids with a variety of applications is formed by oil hydrocarbons oxidation. Synthetic petroleum acids (SPA) are used for syntheses of chemical products, including desiccants, homogeneous catalysts, corrosion inhibitors, surfactants etc [2]. However, in the liquid-phase oxidation process of petroleum hydrocarbons, simultaneously with SPA, oxyacids (OSPA) are also formed in a significant amount, which have wide application in industry. Thereby, the process of obtaining the mixtures of SPA and OSPA could be recommended for commercial implementation, therefore it is necessary optimization of the process by contemporary computer programs.Thus, the aim of this work was studying of liquid-phase oxidation of naphthene-paraffinic hydrocarbons in the presence of the nanostructured reduced graphene oxide (RGO). Diesel fraction of Azerbaijan oil mixtures was taken as an object of study. The fraction was dearomatized. All of the characteristic properties of initial diesel, and also naphthene-paraffinic fractions, separated from it, have been determined. IR-spectra of the samples (before and after dearomatization) were taken on ALPHA İQ-Furye spectrometer, produced by BRUKER company of Germany. Catalytic oxidation process have been carried out in reactor of bubble type by 300 l/kg·h. air speed at 135-140˚C during 5 h. in the presence of different amounts of catalyst. After the oxidation the target products (SPA and OSPA) have been separated from the oxidate according to the known method by precipitation with light benzine or petroleum ester. The results of oxidation process are presented in the table.

Catalyst content, % mas.	Oxidate		SPA		OSPA		SPA+OSPA
	A.n., mgKOH/g	Yield, %	A.n., mgKOH/g	Yield, %	A.n., mgKOH/g	Yield, %	Yield,%
Without catalyst							
0	25,8	80	80,4	5,6	68,2	2,8	8,4
RGO							
0,02	35	82,5	112,8	7,4	100,8	2	9,4
0,05	58,2	96,2	139,5	13	119,5	9	22
0,07	59	96,5	140,8	13,8	120	14,2	28
0,1	66,7	97,3	155	15	115,2	21,2	36,2
0,15	66	96,9	140,5	15	112	17,2	32,2
0,2	63	96,2	141,8	13,2	115	14,1	27,3

As seen from Tab., crude loss in oxidation process is insignificant – the yield of oxidate amounts to ≈96-97%.

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URANIUM AND THORIUM DETERMINATION IN SEA SEDIMENT AND WATER SAMPLES FROM AZERBAIJAN SECTOR OF CASPIAN SEA

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The Caspian Sea is the largest lake on our planet. It is bigger than the Great American lakes and Lake Victoria in Africa by surface area. The present study was conducted to investigate the uranium and thorium contents of sediment and water samples, which were collected from different sites in Azerbaijan region of the Caspian Sea. Uranium and thorium concentration in sediment and water samples from Azerbaijan sector of Caspian Sea has been measured using inductively coupled plasma mass spectrometry (ICP-MS).

It is known the analysis of ultra trace elements in sea water samples is one of the most difficult analytical tasks in the field of environmental monitoring, as extremely low detection limits for elements buried in a highly saline matrix is required. Although the technique of ICP-MS is very powerful by virtue of its sensitivity and selectivity, one of the operational limitations is that of the total amount of dissolved solids which may be introduced into the system. This limitation comes about in part because samples may deposit condensate on the sampler cones over a prolonged analytical run causing signal changes and hence degrading the signal stability. To avoid this problems the Agilent 7700x Series ICP-MS applied to analysis seawater. The Agilent 7700x ICP-MS combines the simplicity of a single collision cell mode (helium mode) for polyatomic interference removal with the superior matrix tolerance of its unique HMI (high matrix introduction) system.

Certified Reference Seawater Probe CASS-5 of the Institute for Environmental Chemistry, Canada, were included to analysis directly after a simple 1+2 dilution with 1% nitric acid, as quality control samples to ensure the accuracy of the results. A reference material, LKSD-2 and LKSD-4 lake sediment samples, supplied by the Geological Survey of Canada was digested with the same acid proportions and analyzed for quality control and a blank sample with the same mixture of acids was processed with each batch of samples.

U concentration in sea water ranged between 6.080-6.714 ug/L, average concentration is 6.333 ug/L. The values of thorium concentration on all sampling point less than 0.01 µg/L. The average concentration of uranium in Caspian Sea water (6.33 ug/L) approximately two times higher than those levels in World Ocean Sea water (2.30 ug/L). The concentrations of the analyzed elements in Caspian Sea sediment were as following: U: ranged from1.115 to 8.546 mg/kg with average concentration 2.375 mg/kg, Th: ranged between 3.70 and 6.948 mg/kg, average concentration 4.536 mg/kg. The Uranium concentration in the analyzed samples was found to be within the crust abundance (< 5 mg/kg) except the four sites which contains slightly higher level of uranium 7.544, 5.489, 7.008 and 8.546 mg/kg respectively. The average abundance of thorium in the Earth’s crust is about 5.6 ppm. In the analyzed samples except the six sites the content of Thorium was found to be within the crust abundance (<5.6 mg/kg).

In general, the Th/U ratio may provide information about the intensity (or index) of weathering and leaching in the sample profile and native, since Th is much less mobile than U. As known the average concentrations of U and Th in sedimentary rocks are 1.2 and 5.97 mg/kg for sandstone, 1.2 and 10.1mg/kg for shales and 1.2 and 1.28 mg/kg for limestone respectively. Using these values, the Th/U ratios are 4.98, 8.42, and 1.07, respectively for the above mentioned rocks types. Also the average world Th/U ratio in deep sea clay is 5.4. The calculated Th/U ratio based on ICP-MS results was found to be from 0.50 to 5.689. This means that the studied sediment samples contain Th/U ratio of natural origin and the one site have higher ratio than 5.4.

EVALUATION OF RAMAN ACTIVE QUALITIES OF DIFFERENT SUBSTRATES IN SERS ANALYSIS OF MORPHINE

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Morphine takes place among the most commonly abused drugs. It can be detected by certain analytical methods; however, cheaper and faster detection tools are studied by forensic and clinical toxicologists. With its' widening application spectrum Raman Spectroscopy and Surface Enhanced Raman Spectroscopy (SERS) rise as a possible alternative tool. There are few studies regarding Raman and SERS spectra of morphine, which are unfortunately controversial. This might be caused by use of different Raman substrates with different Raman active quality. In this study we aimed to compare "Microscope Slide, TLC paper, Silver surface, Gold surface, Gold Nanocellulose surface, Gold Nanocellulose Aniline surface" in order to find out more efficient Raman active substrate for morphine detection.

Morphine, in acetonitrile solution, in concentration of 1 mg/mL was used as sample solution. Morphine solution was dropped as 2 µL on to studied surfaces. After an incubation period of five minutes, 2 µL of colloidal Ag nanoparticles was dropped on sample. Raman spectra gathered by a Raman Spectroscope with 785 nm laser source. Main peaks of morphine was obtained at 627 cm^{-1}. Gathered spectra of morphine have been compared for each studied surface and results are discussed with the related literature.

Keyword: SERS, Raman active substrate, Morphine,

REFERENCE CORRELATION OF THE THERMAL CONDUCTIVITY OF 1-HEXANOL FROM THE TRIPLE POINT TO 600 K AND UP TO 60 MPa

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1-Hexanol is the first member of higher alcohol series, in the plasticizers range, which finds extensive application in the manufacturing of plasticizers and lubricants. Hexan-1-ol is also known for its excellent role as a solvent. The use of 1-Hexanol in industry has made it one of the most important substances for which the development of accurate equations of thermal conductivity is needed.

Based on the most reliable experimental data, the equation for calculation of thermal conductivity of 1-Hexanol has been developed. The thermal conductivity of 1-Hexanol are expressed in this work using the equation

$$\lambda(\rho,T) = \lambda^0(T) + \lambda^r(\delta,\tau) + \lambda^c(\delta,\tau) \tag{1}$$

where λ is the thermal conductivity in $mW \cdot m^{-1} \cdot K^{-1}$, $\lambda_0(T)$ is the dilute gas thermal conductivity, $\lambda_r(\delta,\tau)$ is the residual fluid thermal conductivity, $\delta = \rho/\rho_c$; $t = T_c/T$; $\lambda_c(\delta,\tau)$ is the thermal conductivity critical enhancement. The dilute gas contribution is given by

$$\lambda^0(T) = N_1\left[\frac{\eta^0(T)}{1mkPa\cdot c}\right] + N_2\tau^{t_2} + N_3\tau^{t_3} \tag{2}$$

where η_0 is the dilute gas viscosity in mPa· s.

The residual contribution to the thermal conductivity is given (in $mW \cdot m^{-1} \cdot K^{-1}$) by

$$\lambda^r(\delta,\tau) = \sum_{i=4}^{n} N_i \tau^{t_i} \delta^{d_i} \exp(-\delta^{l_i}) \tag{3}$$

The empirical equation for the residual contribution is similar to the terms used in typical Helmholtz energy equations of state. The number of terms was kept to a minimum to aid in the extrapolation of the equation to low and high temperatures and to high pressures and densities. Nonlinear fitting techniques similar to those employed in [2] were used here to derive the final equation. The thermal conductivity critical enhancement model of Olchowy and Sengers [1] was used to calculate the fluid properties in the critical region.

The proposed equation is valid over all liquid and vapor states, and a simplified cross-over equation was used to model the behavior of the critical enhancement. The proposed equation can be applied over a temperature range from the triple point to 600 K with pressures up to 60 MPa. The uncertainties of calculated values from the equation are generally within 2%. The proposed equation correctly reproduce the surface of state and allow the calculation of thermal conductivity with sufficient accuracy.

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THERMOPHYSICAL PROPERTIES OF BINARY 1-BUTYL-3-METHYLIMIDAZOLIUM HEXAFLUOROPHOSPHATE + METHANOL MIXTURES

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Ionic liquids (ILs) are a salt in the liquid form. They are potentially "green" replacements for conventional organic solvents, because they have negligible vapor pressure, nonflammable, thermal stable, and recyclable properties. Ionic liquids and their organic mixtures are interesting to be useful as heat transfer fluids in absorption refrigerating and solar heating systems.

This work is a continuation of our investigations in the field of (p,ρ,T) properties of ILs and alcohol solutions. The new accuracy (p,ρ,T) data of 1-butyl-3-methylimidazolium hexafluorophosphate + methanol mixtures at the wide range of temperature T=(278.15 to 413.15) K and pressures up to p=140 MPa are reported with an estimated experimental relative combined standard uncertainty of $\Delta\rho/\rho$= ±(0.01 to 0.08) % in density, which were investigated using a Anton-Paar DMA HPM vibration-tube densimeter. Measurements were made for 10 concentrations from x=(0 to 1) mole fraction of methanol (x=0.0000, 0.1537, 0.3289, 0.5675, 0.7599, 0.8601, 0.9006, 0.9442, 0.9728, 0.9899, 0.9947 and 1.0).

The density values $\rho(p_0,T)$/kg·m^{-3} at ambient pressure and at temperatures T = (273.15 to 413.15) K were investigated using the combination of the Anton Paar DMA 5000M, DSA 5000M and DMA HPM vibration tube densimeters with an uncertainty of $\Delta\rho$ = ± (5·10^{-3} to 3·10^{-1}) kg·m^{-3}. The speed of sound values $u(p_0,T)$/m·s^{-1} at ambient pressure and temperatures at T = (283.15 to 343.15) K are investigated using the Anton Paar DSA 5000M vibration tube densimeter and sound velocity meter with intervals of ΔT= (5-10) K and an uncertainty of Δu= ± 0.1 m·s^{-1}.

An empiric equation for fitting of the density values of [BMIM][FAP] and methanol mixtures has been developed as a function of pressure, temperature and mole fraction of methanol. The excess molar volumes V_m^E /cm^3·mol^{-1} and apparent molar volume V^F /cm^3·mol^{-1} of the investigated mixtures were calculated using the pure components and mixture properties.

Keywords: Ionic liquid, density, excess molar volume, apparent molar volume, thermophysical properties.

THE STRUCTURAL AND VIBRATIONAL PROPERTIES OF $CuFe_{0.99}Ni_{0.01}S_2$

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$AB^{III}C_2^{VI}$ (A – one-valent cations, B − three-valent cations, C – chalcogen) triple chalcogenide compounds is a less studied compounds providing various physical properties. One of the most studied compounds in these compounds is a chalcopyrite $CuFeS_2$ compound. It has an extensive forbidden zone of the semiconductor properties, converts it to signifcant material for electronica and spintronica. In this work, there were conducted partial replacements of Fe^{3+} ions with Ni^{3+} ions in chalcopyrite $CuFeS_2$ crystals. The crystalline structure and atomic dyanmics of obtained $CuFeS_2$ and $CuFe_{0.99}Ni_{0.01}S_2$ compounds were studied.

$CuFeS_2$ and $CuFe_{0.99}Ni_{0.01}S_2$ compounds were synthesized by alloying elements of specific purity: carbonyl Fe and Ni, electrolytic copper – M0, OSCh 19-5 grade sulfur. The alloying was performed in evacuated (~ 0.1 Pa) quartz ampoules in divariant conditions. The partial pressure of volatile component was regulated by changing the temperature in the cold part of the ampoule. At the beginning of the process, the temperature of the high-temperature part of the ampoule was gradually raised up to 1100 °C, while a part of the unreacted sulfur condensed in the cold part of the ampoule and was consumed as the synthesis proceeded. At the end of synthesis temperature of the cold part of ampoule was 450 °C; partial pressure of sulfur was over than 1 atm. After 6 hours of synthesis, the rate of cooling ampoule was 10 grad/min. Obtained samples were ground into powder and pressed at 200 atm, after that they were roasted at 700 °C during 200 hours.

The X-ray diffraction measurement was performed using a Bruker D8 Advance powder diffractometer with the following parameters: 40 kV, 40 mA, Cu Kα radiation (λ = 1.5406 A). The X-ray diffraction data were treated using the FullProf program. The Raman spectra were measured using a LabRam spectrometer (NeHe laser with wavelength 633 nm, confocal slit 110 μm, ×50 lens).

It was determined that, $CuFeS_2$ having tetragonal structure I-42d spatial groups in normal condition, lattice parameters: corresponds to a = 5.2904(5) Å, c = 10.4266(1) Å points and this compatible to the previous results. It was found that, the obtained $CuFe_{0.99}Ni_{0.01}S_2$ compounds in normal condition having I-42d spatial group of partial replacement of Fe atoms of $CuFeS_2$ with Ni atoms almost there is no difference in points of lattice parameters and atom coordination. This compliance, occurs regarding to having ion radius familiar to Fe^{3+} ions (r_{Fe} = 0.623 Å) Ni_{3+} ions (r_{Ni} = 0.623 Å).

Obtained spectra by Raman spectroscopy in 100-700 cm-1 interval at room temprature of $CuFeS_2$ and $CuFe_{0.99}Ni_{0.01}S_2$ compounds. It seems from spectrs by Raman spectroscopy that, there are observed 3 various maximum of $CuFeS_2$ compounds: $v_1 = 210$ cm^{-1}, $v_2 = 274$ cm^{-1}, and $v_1 = 387$ cm^{-1}. These modes corresponds to rejimes in theoretical calculation $v_1 = 189$ cm^{-1}, $v_2 = 270$ cm^{-1}, and $v_1 = 383$ cm^{-1}. When the Ni atoms entered into compounds, there observed fundamental changes in Raman spectrs. It seems from spectrs, observed two mode having $v_1 = 258$ cm^{-1} və $v_1 = 283$ cm^{-1} points. The morphology studies that sizes magnified ×50 times shows that, Ni atoms entering to these compounds, increases the brightness of the samples. Here we come to the conclusion that, upon replacement of Fe atoms partially with Ni atoms, observed optical activity and there can be observed only faint $v_1 = 258$ cm^{-1} mode in $v_1 = 283$ cm^{-1} mode background corresponds to NiS_4 tetraedr vibration.

DENSITY OF THE KURA RIVER WATER

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Kura river (total length is 1515 km) starting in north-eastern Turkey, it flows through Turkey to Georgia, then to Azerbaijan, where it receives the Aras River as a right tributary, and enters the Caspian Sea. Pollution of the river from the territory of the neighbouring states creates an environmental tension. Mineralisation of the water of the Kura river raises till 800-1200 mg in the connecting part of Araz and Kura rivers is 35-50 per cent more compared to its medium current. Density of polluted water of Kura river is max. 9 times more than sanitary norms. More than 350 million m^3 of the chemically and biologically polluted water annually injects the Kura river pool. From this point of view, it is important to conduct, from the security of the population point of view, a general monitoring over the dangerous substances in the transborder rivers.

During our last research activities, we have investigated the thermophysical properties (density, vapor pressure, viscosity, speed of sound, chemical compounds analysis) of 14 Kura river water sample in Azerbaijan side from west to east over the parameter range of interest. In this presentation, we will inform the the thermophysical properties of four new water samples of Kura River in Turkey side from its source at Ardahan region, which are carry out at DMA HPM high pressure – high temperature vibration tube densimeter. The density and speed of sound measurements at ambient pressure are carry out using the DSA 5000M density and speed of sound measurement installation. The chemical compounds analysis using the IRIS Intrepid II Optical Emission Spectrometer and DX 100 ion chromatography are also presented. These investigations have been examined for the first time. The comprehensive and accurate thermodynamic equation of state over a well specified range of parameters which are of interest in ecological research are constructed, which are used to calculate thermophysical properties of these samples. Using the (p,ρ,T) data, the comprehensive and accurate thermodynamic equation of state over a well specified range of parameters which are of interest in ecological research was constructed, which is used to calculate thermophysical properties of these samples.

BIODEGRADABLE ANIONIC ACTIVE SURFACTANTS ON THE BASIS OF POLYUNSATURATED FATTY ACIDS

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In the countries of well-developed oil and petrochemical industries, accidents and other unforeseen circumstances are practically inevitable both at production, transportation and processing of oil. As a result, hydrosphere is polluted. The oil spilled on water surface, in many cases removed mechanically. However, mechanically removing of the thin oil film from water surface fails. In these cases, special types of surfactants are used which should have oil-collecting and oil-dispersing properties. Simultaneously, they should be environmentally safe. Therefore, it was interesting studying of the biodegradability of anionic active (anionic) surfactants having oil-collecting and oil-dispersing properties obtained on the basis of both individual fatty acids and mixtures of fatty acids, extracted from vegetable oils.

As polyunsaturated fatty acids, it has been used linolenic acid (LA) - monocarboxylic acid with three isolated double bonds and acids derived from vegetable oils. For the preparation of the mixture of unsaturated fatty acids, corn oil has been taken (CO) and a mixture of fatty acids has been selected from it by the saponification and subsequent treatment by hydrochloric acid. In the hydrolysis process, triglycerides in the oil are converted into sodium soaps. Thereby glycerin is formed as a by-product.

The resulting acid mixture has been used without further separation. The acids, separated from corn oil and also linolenic acid have individually been sulfated with the solution of sulfuric acid. The structure of the products obtained has been proved by Fourier transform infrared spectroscopy (FTIR). Some properties of sulfated fatty acids have analytically been determined.

It has been taken 10% of calcium chloride salt for the preparation of the calcium salt and mixed with the sulphonic acids in a ratio of 2 : 1 at room temperature. The calcium salt of sulfonic acid is insoluble in water and separated by filtration.

It has been defined elemental and chemical composition of anionic surfactants on the base of LA by X-ray fluorescence microscopy. Elemental analysis of the samples have been carried out by using of X-ray microscope XGT-7000, Horiba with accelerating voltage of 50kV X-ray tube, falling X-ray beams diameter is 100 mkm , measuring time -60 seconds.

The reaction products were characterized by ^{1}H NMR spectroscopy (Model BRUKER) in the frequency range of 400 MHz, solvent DMSO-D$_6$, standard - GMDO. The chemical structure of the fatty acids separated from corn oil and sulfated acids were characterized by physico- chemical and spectroscopic methods. Infrared spectra were taken using FTIR, spectrometer Bruker with KBr discs using a frequency range 4000-500 sm^{-1} as well as on the device (Perkins Elmer) Spectrum BX, range 4200-400 sm^{-1} .

Oil-collecting properties of anionic surfactants (calcium salts of sulfonic acids) have been studied by the example of oil deposits of Ramany oil field of Absheron peninsula (Azerbaijan). Density 0.86 g / sm^3; kinematic viscosity at 20^{0}C - 16 mm^2/s. Surfactant or its solution (5-10 % solution in ethanol) has been added to the thin oil film (the thickness of 0.16-0.17 mm) in Petry cup.

Tests for detecting of biodegradation of anionic surfactants have been carried out as follows: the filtered samples (solutions in river water) has been prepared daily or at certain time intervals and determined by interfacial tension on the border of water: kerosene phase. The microflora of river water (Geychay, Azerbaijan) in species composition consisted mainly of adapted to permanent residence of the following bacteria: Chromobacterium Violaceum, Bacterium Aquatilis, Mikrococcus Candicans, Pseudomonas Fluorescens and Mikrococcus Roseus The amount of bacteria in pure river water does not exceed 100 -120 кl in 1 ml. and on the surface of different water (distilled, freshwater and seawater).

As a result of the investigations, it has been found out that the synthesized calcium salts on the basis of acid extracted from corn oil and linolenic acid have good oil-collecting and oil-dispersing properties in all test environments (drinking, distilled, sea water) in a diluted form, and capable of holding a thin oil film within 70 up to 166 hours. Synthesized calcium salts based on individual LA and the mixtures of fatty acids extracted from the CO undiluted in distilled and fresh waters have a low oil-collecting capacity.

The highest oil collecting coefficient are observed in seawater 88.5 - for a mixture of acids and 90.2 - for calcium sulfate of linolenic acid. At the concentration of salts in ethyl alcohol 5 and 10% oil-collecting properties of salts are improved. At the concentration of 10% linolenic acid, calcium sulfate oil-collecting coefficient in freshwater is 93.3. Reagent is active for 6-7 days. Thus, it has been found that anionic surfactants - calcium sulfate on the base of ZhK mixture extracted from CO and calcium sulphate based on LA have strong oil-collecting and dispersing properties towards the thin oil films on water surfaces.

Thus, as a result of the researches, it has been found that, oil-collecting and oil-dispersing reagents, capable of degrading in the environment on environmentally safe compounds may be obtained on the basis of Ca-salts of sulfated fatty acids (a mixture of acids selected from the CO and LA). It has been found that the most hydrophobic molecules of anionic surfactants are decomposed at first.

THERMAL INVESTIGATION OF REDOX RICH TIN(IV) COMPLEXES BASED ON FERROCENE-CONTAINING O-BENZOQUINONATO LIGANDS

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Electron-transfer reactions play an important role in a variety of chemical and biological processes. One of the most prospective and interesting concepts is the study of metallocene – *o*-quinone dyads. The ability of ferrocene and redox-active quinoid type ligands to the reversible oxidation makes such objects to be promising system for the study inter- and intramolecular electron transfer (ET) between the *o*-benzoquinone ligand and ferrocene.

The interaction of bis-o-benzosemiquinonato chlorine-containing tin(IV) complexes with ferrocene in molar ratio 1:1 in acetonitrile gives ET complexes of $[(SQ)(Cat)SnCl_2]^{-}Fc^{+}$ type (Scheme 1). It was found, that this ionic complexes, depending on the substituent, demonstrate different magnetic exchange between paramagnetic centers (ferrocenium-SQ ligand) in low temperature.

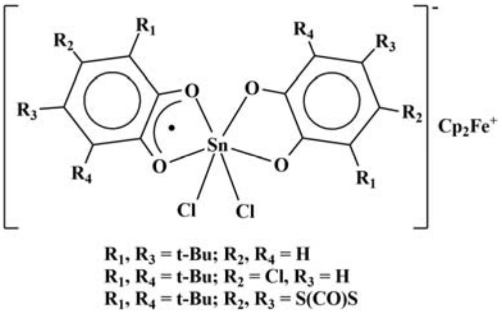

Figure 1.

The novel tin(IV) ET complexes were characterized by means of IR-, UV -spectroscopy, X-ray, magnetochemistry and thermal analysis. Differential scanning calorimeter DSC 204F1 Netzsch was used for measuring heat capacity of complexes in temperature range 150-650 K in nitrogen atmosphere and heating rate 5 K/min.

Acknowledgements: We are grateful to RFBR (grant № 16–03–00700a) for financial support.

THERMAL INVESTIGATION OF COBALT(II, III) COMPLEXES BASED ON FERROCENE AND O-BENZOQUINONE TYPE LIGANDS

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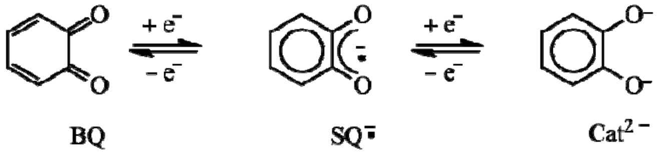
Recently, the intensively developing region of chemistry - coordination chemistry of transition metal complexes based on redox active ligands such as o-quinones attracts an attention of researchers in the fields of fundamental and applied science. Interest to these compounds is caused mainly by the fact that the redox active ligands are capable of reversibly oxidizing or reducing being in the coordination sphere of the metal. On the other hand, ferrocene as well as redox-active ligands are able to the reversible oxidation, and can form complexes with charge transfer in systems with an electron-withdrawing moiety. The combination of transition metal, redox active ligand and ferrocene in one molecule is the great interest in the formation of new types of o-quinone complexes; and is the promising system in terms of electron-transfer interactions.



The novel type cobalt(II) complex based on Schiff ligand containing ferrocene-aldimine substituent was synthesized and characterized by IR spectroscopy, chromato-mass spectrometry and thermal analysis. In accordance with EPR spectroscopy the oxidative addition of o-benzoquinones to cobalt(II) bis-o-iminophenolato complex in the molar ratio of 1:1 in toluene gives o-benzosemiquinonato cobalt(III) complex (Scheme 1).

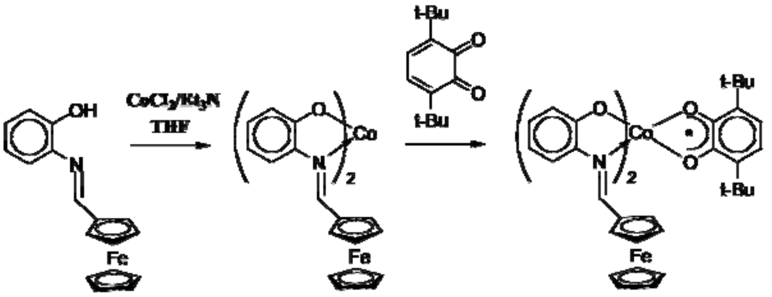


Figure 1.

Differential scanning calorimeter DSC 204F1 Netzsch was used for measuring heat capacity of complex in temperature range 150-650 K in nitrogen atmosphere and heating rate 5 K/min.

Acknowledgements: The reported study was funded by RFBR according to the research project № 18-33-00951 mol_a

O,O-DIALKYLARYLDITHIOPHOSPHATES OF METALS AS AN ANTIOXIDANT AND ANTICORROSION ADDITIVES

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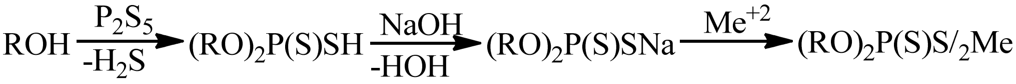
It is known that metal-containing dithiophosphates are widely used as additives for motor oils, stabilizators of polymers, agents of vulcanization of rubber and rubber products, flotation agents and etc.

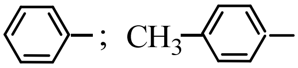
The synthesis of same compounds carrying out by phosphorosulfuration of organic compounds containing hydroxyl groups, in particular, alcohols and phenols, and also other compounds, having labile hydrogen atom with phosphor pentasulfide with further transfer of obtaining dithiophosphoric acids by exchange reaction with inorganic metal salts with receiving of metal complexes of this acids.

The reaction was carried out in glass reactor, equipped with supply line of start materials, a stirrer, a reflux condenser and a discharge line, obtaining as the result in the reaction of H_2S and the capacity to neutralize to latter. The scheme of reaction is as follows:



$$ROH \xrightarrow[-H_2S]{P_2S_5} (RO)_2P(S)SH \xrightarrow[-HOH]{NaOH} (RO)_2P(S)SNa \xrightarrow{Me^{+2}} (RO)_2P(S)S/_2Me$$

where, R- C_2H_5; i-C_3H_7; i-C_4H_9;



Me– Ni, Co, Cu, Cr

Synthesized metal complexes of O,O-dialkyl(aryl)dithiophosphates of metal, especially Ni and Co complexes were shown a high effectively as an antioxidant and anticorrosion additives to oils, polyfunctional stabilizers of polyolefin, against their heat and light degradation as well as the components of the catalyst systems in the preparation of low and high molecular weight of polybutadiene.

EFFECT OF ANNEALING CONDITIONS ON METAL INSULATOR TRANSITION OF SPUTTERED VANADIUM OXIDE

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Vanadium oxide is a promising candidate that exhibits a dramatic change in its electrical conductance by a structural phase transition from insulating monoclinic to metallic rutile upon either direct heating or optical pumping. The increase in carrier density changes the refractive index dramatically. This phenomena could be used to desing and fabricate tunable optical structures, thermochromic coatings for intelligent windows, optical triggers for ultra fast data tranport applications, tunable plasmonic nano antennas.

In literature its shown that many forms of Vanadium oxide exists such as VO_2, V_5O_9 and V_2O_3. Thin films which are deposited by sputtering are mixtures of all that forms. Phase transition order depends on the relative ratio of the VO_2 species. The higher VO_2 ratio means, higher phase transition magnitude. Reactive sputtering by adding O_2 in sputtering atmosphere, and in-situ annealing are the most used methods to overcome the issue. Alternatively post anneling method is used for increasing both the cristal quality and phase trasition magnitude of the films.

In this work, VO_2 thin film with 80 nm thickness has been deposited onto a c-plane sapphire wafer with a VO_2 target under nonreactive environment (only Ar atmosphere) by using RF magnetron sputtering system. After the deposition; parametric annealing trials have been carried out according to the variation of Ar and O_2 gas ratio. Among annealing conditions with 5:1, 10:1 and 20:1 Ar/O_2 gas ratio parameters, maximum transition is observed for annealing condition with 20:1 Ar/O_2 gas ratio. To show the electrical resistance change temperature dependent four-probe measurements have been done. For the sample observed maximum electrical resistance change; transition temperature is nearly 340 K and max./min. resistance ratio is in the order of nearly 1.5E+3 and hysteresis loop has been observed.

QUANTUM COMPUTATIONAL STUDIES, SPECTROSCOPIC (FT-IR, FT-Raman, NMR and UV-Vis) PROFILING ON 1,3,4-Thiadiazole-2,5-Dithiol

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The research exploration will comprise of investigating the molecular structure, vibrational assignments, bonding and anti-bonding nature, nonlinear optical, electronic and thermodynamic nature of the molecule. The research is conducted at two levels: First level employs the spectroscopic techniques -FT-IR, FT-Raman and UV–Vis characterizing techniques; at second level the data attained experimentally is analyzed through theoretical methods using and Density Function Theories. A comparison is drawn between the two levels and discussed. The probability of the title molecule being bio-active theoretically proved by the electrophilicity index leads to further property analyzes of the molecule. The results of the organic amine 1,3,4-Thiadiazole-2,5-dithiol is analyzed and discussed.

The calculations were performed at DFT levels by using Gaussian 09 [1-2] program package, invoking gradient geometry optimization [3-4]. The optimized structural parameters were used in the vibrational frequency calculations at the DFT level to characterize all stationary points as minima. Then, vibrationally averaged nuclear positions of title compund were used for harmonic vibrational frequency calculations resulting in IR and Raman frequencies. In the present work, the DFT method B3LYP with 6-311G(d,p) basis set were used for the computation of molecular structure, vibrational frequencies and energies of optimized structures. The vibrational modes were assigned on the basis of TED analysis for 6-311G(d,p) basis set, using SQM program [5].

Keywords: 1,3,4-Thiadiazole-2,5-dithiol, Molecular structure, Vibrational spectra, Density Functional Theory (DFT)

Acknowledgments: This study was supported by Gazi University Scientific Research Projects Department (BAP project code: 05/2018-06).

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THERMODYNAMIC PROPERTIES OF $Ag_8Ge_{1-x}Mn_xTe_6$ ALLOYS

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The ternary Ag_8GeTe_6 compound is characterized by a polymorphic transformation. Due to the complex crystal structure and large size of a unit cell this compound has many unusual properties; it exhibits low thermal conductivity and a small energy band. In addition, Ag_8GeTe_6 is a promising material with thermoelectric characteristics above 500K temperature and super ionic conductivity. The strong changes in the kinetic parameters at the phase transitions allow them to be used in electrical switches, voltage amplifiers and other transducers.

By alloys, based on the Ag_8GeTe_6 compound, it is possible to change or adjust its parameters and phase transitions temperatures. Due to the fact that the manganese impurities have a high solubility and diffusion ability, its addition makes it possible to regulate the structure and properties of the material.

Solid solutions $Ag_8Ge_{1-x}Mn_xTe_6$ (x = 0, 0.01, 0.02, 0.05, 0.1) were prepared by fusing high-purity elements at a temperature of 1200K and cooling to room temperature. Then the samples were homogenized at ~500K temperature for 48 hours.

X-ray phase analysis of the samples was carried out using Broker D2 Phaser instrument. The diffractograms of Ag_8GeTe_6 compound and the solid solution $Ag_8Ge_{1-x}Mn_xTe_6$ (x = 0.1) showed in Figure 1. The change in the interplanar distance was indicated in figure only for four angles. The analysis showed that structures of the synthesized system have those of Ag_8GeTe_6 compound, however, the reflexes of the composition containing 10% manganese insignificantly shift toward small angles (Table), i.e. the introduction of manganese atoms leads to the compressed of the lattice.

Differential scanning calorimetric studies in argon atmosphere were carried out using "NETZSCH DSC 204F1" instrument (Germany) in the 100-900 K temperature range. The heating rate was 10K/min, the inert gas velocity was 20ml/min. The endothermic transformations are observed at the 182K, 227.8K, 245K, 339.6K, 626K for the x=0.05 and at 227.6K 248K 627K temperatures for x=0.1 composition (Fig.2). The specific heat of the samples was determined from the temperature dependence of the heat flux (Figure 3) and, in turn, entropy (S=0.223J/gK), the enthalpy (H=40.545 Jg) and the Gibbs energy (G=-26.261Jg) were determined from the heat capacity data.

Table. The interplanar distance for $Ag_8Ge_{1-x}Mn_xTe_6$.

d, x=0	3.48534	3.33707	2.22531	2.04417	1.95455	1.76336	1.50528	1.32629
d, x=0.1	3.48256	3.33463	2.22433	2.04316	1.95169	1.76182	1.50416	1.32579
D d	0.00278	0.00244	0.00098	0.00101	0.00286	0.00154	0.00112	0.0005

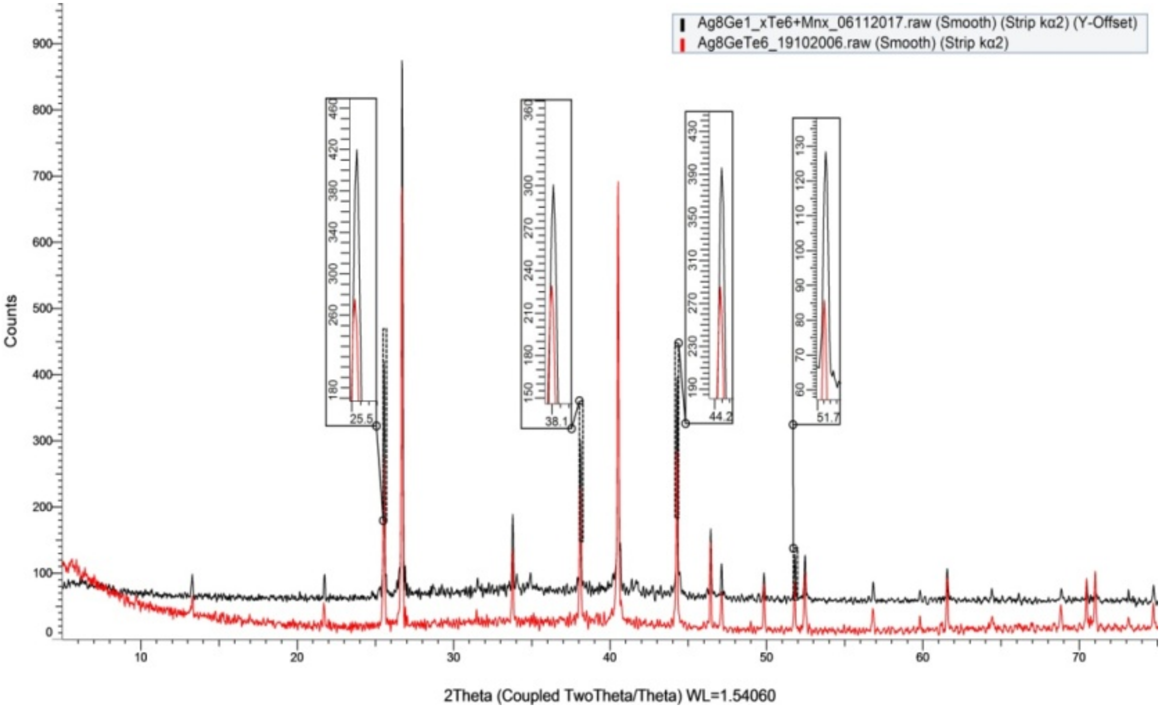

Figure 1. X-ray diffraction pattern of $Ag_8Ge_{1-x}Mn_xTe_6$ (x=0; x=0.1)

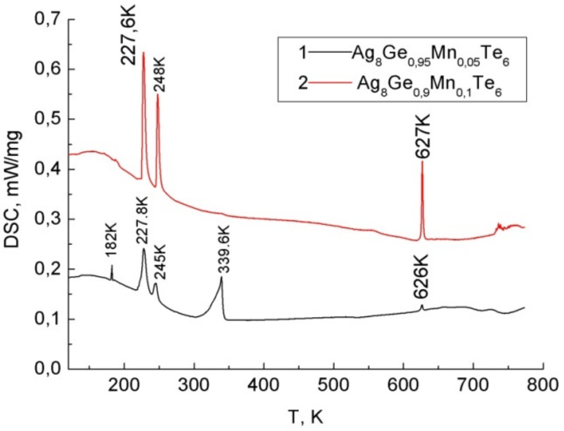

Figure 2. Heat flow versus temperature for $Ag_8Ge_{1-x}Mn_xTe_6$ (x=0.05; x=0.1)

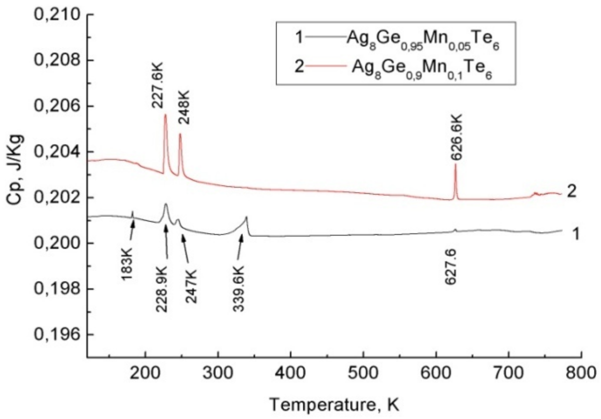

Figure 3. Heat capacity of $Ag_8Ge_{1-x}Mn_xTe_6$ (x=0.05; x=0.1) solid solutions.

MICROSCALE THERMOPHYSICS GROUP: A REVIEW OF INVESTIGATIONS

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The description of a substance behavior under the influence of a heat release is convenient to carry out for quasi-static conditions of heating or cooling. For this, it may be sufficient to know the temperature dependence of thermophysical properties and the values of phase transition temperatures for a given pressure. The properties of fluids in absolutely stable states, at least for pure liquids, have been investigated rather well. Generally, these properties may be repeatedly measured, since reliable experimental methods have been developed for such states [1]. However, in practical applications the temperature values of working fluids do not confined within a stable states range. For example, the range of stable states of liquid phase for water at atmospheric pressure extends, taking into account the phenomena of attainable superheat (310℃) and supercool (−40℃), up to 3.5 times (due to so-called not fully stable states [2]).

In our report, the attention will be paid to not fully stable fluids under high-power heating or pressure drop. We shall use the term “not fully stable fluids” to refer to fluids that reduce stability in the course of heating or pressure drop (superheated liquids), as well as initially relatively stable systems (nanofluids and supercritical ones). We shall use the term “superheated liquids” to refer to liquids superheated with respect to the liquid-vapor or liquid-liquid equilibrium temperature and the temperature of thermal decomposition onset in quasi-static process. Because of the obvious experimental difficulties, the properties of these fluids are less studied. Moreover, a search of suitable methods for solving this problem is still in progress [2, 3].

Research methods: the technique of controlled pulse heating of a wire probe [2, 4] and the technique of optical fibre-based sensor placed in a miniature bubble chamber with constant temperature [3, 5]. Research objects: pure liquids (from simple liquids to polymeric ones), mixtures (including oils), nanofluids and supercritical fluids.

Main lines in research: attainable superheat and critical parameters of fluids; short-term thermal stability of oils and polymers; effect of water admixtures on thermal stability and heat transfer in oils; heat conduction in nanofluids and supercritical fluids at small time and spatial scales; density of superheated liquids; thermal conductivity of liquids [6]; microoptical investigation of mechanism of spontaneous boiling-up onset.

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CALCULATION OF THERMOPHYSICAL PARAMETERS OF LAYERED COMPOUNDS InGaSe2

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The calculation of the thermophysical parameters of $InGaSe_2$ crystal based on the density functional theory (DFT) is performed. The literature contains information on the properties and band structure of a ternary compound $InGaSe_2$ [1-3].

It is known that analyzing such thermodynamic parameters as entropy, enthalpy and free Gibbs energy, one can obtain information about the nature of the chemical bond in semiconductors. The thermodynamic characteristics of the compounds are also used in testing various models of interatomic forces. Obtaining detailed data of thermodynamic functions for a particular solid state is an independent scientific and applied interest. As is known, the total average energy of the system is determined by the expression [4].

$$\overline{E} = \int_{\omega_{\min}}^{\omega_{макс}} g(\omega)\overline{\varepsilon}(\omega)d\omega = \int_{0}^{\omega_{макс}} \left(\frac{3}{2\pi^2}\right)\left(\frac{\hbar\omega^3}{\vartheta^3}\right)\frac{d\omega}{e^{\hbar\omega/\kappa T}-1},$$

where g(ω) is the spectral density, g(ω) dω is the number of modes in the interval from ω to ω + dω. Using the expression, one can find the internal energy of a solid state body and then differentiating the result obtained, determine the heat capacity and other thermophysical parameters associated with them (fig.). According to the frequency dependence of the heat capacity (C_V) thermophysical parameters ternary compound were calculated. The calculation results are shown in the figure.

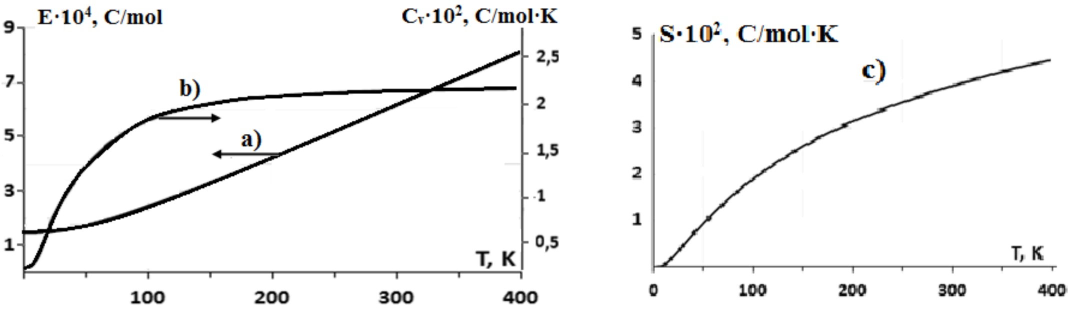

Fig. The temperature dependences of total energy (E) (a), the specific heat at a constant volume (b), and the change in the molar entropy (c) of the compound $InGaSe_2$

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SURFACE MICRORELEFF AND TEMPERATURE CHARACTERISTICS OF DIELECTRIC PARAMETERS OF *LDPE*+x vol% Bi_2Te_3 COMPOSITES

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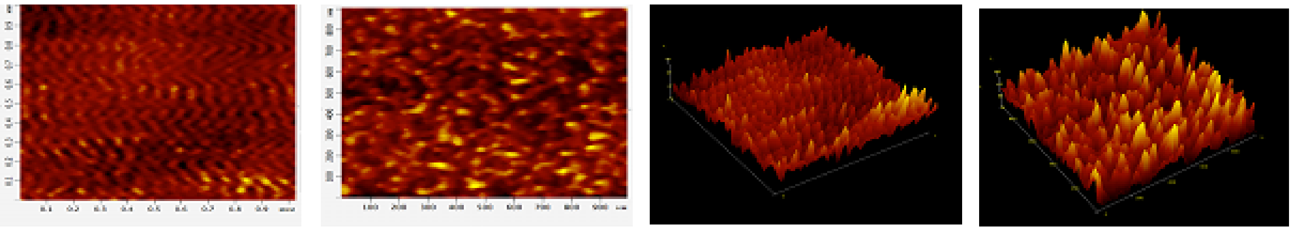
Microscopic particles and formations on surfaces of composites, *LDPE* - low density polyethylene mixed with wide application capabilities - Bi_2Te_3 compound, were studied by atomic force microscope on *2D* and *3D* scales. Analysis of the results given in Figure 1 shows that, as the increase in the amount of composites containing Bi_2Te_3 semiconductor compound order on their surfaces liked as observed in crystals. Figure 2a describes the variations of the dielectric properties of these composites depending on the temperature at the temperature range $20 \div 150^0C$. The results indicate the weak increasing of ε (T) dielectric permeability of composites containing 3 to 10 wt% fillers, and in composites with 15 and 20 wt % fillers observed a weak minimum at 100^0C. Temperature dependencies of the dielectric loss angles of *LDPE*+ volume% Bi_2Te_3 composites are given in Figure 2b. As shown in the figure, tgδ (T) is practically constant even though the amount of additives in the *LDPE*+ wt% Bi_2Te_3 composites is x = 3 ÷ 10, but tgδ (T) line decreases by law in composites of 15, 20 wt %. With the increase in amount of filler the tgδ (T) increases. Depending on the amount of filler, the changes of ε (T) and tgδ (T) are related to Maxwell-Wagner polarization of composites.



a) **b)** **c)** **d)**

Fig 1. AFM-images of *LDPE+wt%* Bi_2Te_3 composite surfaces in *2D* and *3D* : a) *LDPE* + 50% Bi_2Te_3 (*2D*); b) *LDPE* + 40% Bi_2Te_3 (*2D*); c) *LDPE* + 50% Bi_2Te_3 (*3D*); d) 60% *LDPE* + 40% Bi_2Te_3 (*3D*)

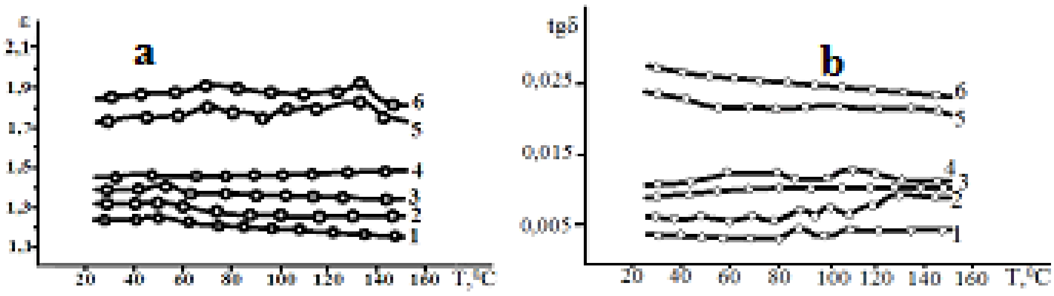


Fig 2. Temperature dependencies of dielectric permeability and dielectric loss angles of composites *LDPE+wt%* Bi_2Te_3: 1- x = 3; 2- x = 5; 3- x = 7; 4- x = 10; 5- x = 15; 6- x = 20.

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TRANSPORT PROPERTIES OF *n*-UNDECANE AND *n*-TRIDECANE

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Normal undecane and normal tridecane, which are the representatives of the homologous series of n-alkanes, relates to technically important hydrocarbons for which reliable data on their transport properties in a wide range of state parameters are required. Such data are used in calculating heat-and-mass transfer equipment, transport systems, and power installations. Furthermore, these substances are often important components in surrogate mixtures for many jet fuels. In this work, we survey the available data for viscosity and thermal conductivity and provide wide-ranging correlations for both transport properties.

We represent the viscosity η of a pure fluid as the sum of a dilute gas contribution and a residual term [1].

$$\eta(\rho,T) = \eta^0(T)[1 + B_\eta(T)\rho] + \Delta\eta(\rho,T) \tag{1}$$

where the term $\eta^0(T)$ represents the viscosity in the limit of zero density, $B_\eta(T)$ is the second virial coefficient for viscosity based on Rainwater-Friend theory, and $\Delta\eta(\rho,T)$ is the residual contribution that represents the higher-order density terms as a function of the absolute temperature and density. This formulation of the viscosity is expressed in terms of density and temperature and requires that the density be available. In this work, we use the equations of state developed by authors [2] to obtain density values.

Expressions for the viscosity in the limit of zero density and for the second viscosity virial coefficient were taken from [2, 3]. We expressed the higher density terms $\Delta\eta(\rho,T)$ of eq 1 in terms of the reduced density and the reduced temperature. After systematic consideration of the alternative structures, the final correlation contains the following combination of polynomial and free-volume terms

$$\Delta\eta(\rho,T) = \sum_{j=2}^{4}\sum_{k=1}^{5}\alpha_{jk}\frac{\delta^j}{\tau^k} + \mathrm{c}_1\delta[1/(\delta_0 - \delta) - 1/\delta_0] \tag{2}$$

The reduced close-packed density is written as

$$\delta_0 = c_2 + c_3\tau^{1/2} + c_4\tau \tag{3}$$

The primary data were used to establish the coefficients of the high-density contribution (eqs. 2 and 3), which are presented in the full-text report.

We represent the thermal conductivity of a pure fluid as a sum of three contributions:

$$\lambda(\rho,T) = \lambda^0(T) + \lambda^r(\delta,\tau) + \lambda^c(\delta,\tau) \tag{4}$$

where λ is the thermal conductivity in mW·m^{-1} ·K^{-1}, $\lambda_o(T)$ is the dilute gas thermal conductivity, $\lambda_r(\delta,\tau)$ is the residual fluid thermal conductivity, $\delta = \rho/\rho_c$; $t = T_c/T$; $\lambda_c(\delta,\tau)$ is the thermal conductivity critical enhancement. The dilute gas contribution is given by

$$\lambda^0(T) = N_1\left[\frac{\eta^0(T)}{1 mkPa\cdot c}\right] + N_2\tau^{t_2} + N_3\tau^{t_3} \tag{5}$$

where η_0 is the dilute gas viscosity in mPa· s.

We used a polynomial in temperature and density to represent the background, or residual, contribution to the thermal conductivity

$$\lambda^r(\delta,\tau) = \sum_{i=4}^{n} N_i\tau^{t_i}\delta^{d_i}\exp(-\delta^{l_i}) \tag{6}$$

The thermal conductivity critical enhancement model of Olchowy and Sengers [4] was used to calculate the fluid properties in the critical region. The number of terms was kept to a minimum to aid in the extrapolation of the equation to low and high temperatures and to high pressures and densities. Nonlinear fitting techniques similar to those employed in [5] were used here to derive the final equation.

The proposed equations can be applied over a temperature range from the triple point to 700 K with pressures up to 100 MPa. The uncertainties of calculated values from the equation are generally within 2 – 2,5 % for viscosity and 1,5 – 2,0 % for thermal conductivity for both substances. The proposed equations correctly reproduce the surface of state and allow the calculation of viscosity and thermal conductivity with sufficient accuracy.

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DENSITY MEASUREMENTS OF N.BUTANOL+ BENZENE IN THE TEMPERATURE RANGE FROM 290 K TO 560 K AND AT PRESSURES UP TO 60 MPa

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The density of n.butanol at atmospheric and high pressure have been reported. There are also reliable data in the literature for the density of benzene. The literature also contains measurements of the viscosity, speed of sound, heart capacity and density for mixtures of alcohols with hydrocarbon.

We have measured the (p,ρ,T,x) of n.butanol and benzene at temperatures T=(290-560) K and pressures p=(0.1-60) MPa. Densities were determined with a magnetic suspension densimeter. That has been described in detail elsewhere [1,2] with an uncertainty of ±0.1%. Only the important features are described here. The sinker was formed from a silver steel of volume 0.2647 cm^3, attached by a brass thread of volume 0.0039 cm^3 a to a solid quartz float of volume 3.1212 cm^3. The mass of the pendant system in vacuum was 8.9650 g. The core silver steel contained a magnetic core of diameter 2 mm and height 85.4 mm. The magnetic suspension is maintained at room temperature by flowing water through a heart exchanger located between magnet and measurement cell. Temperature was measured with a platinum resistance thermometer with an accuracy of 0.01 K. The temperature of the magnetic suspension was measured with mercury-in-glass thermometers with a precision of 0.1 K.

A detailed analysis of the concentration dependence of (p,ρ,T,x) data of studied systems has shown, that concentration dependence of the density deviates from the additive it line and changes with temperature and pressure. The analysis of the given experimental shows that for all the substances investigated the equation of state proposed by Naziyev and Hasanov is suitable:

$$\rho^4 = A + B\cdot p^{0.5} + C\cdot p \tag{1}$$

where p is the pressure, MPa; ρ is the density of substance, g/cm^3; A, B, C are the temperature (T, K) dependent coefficients. The A, B, C coefficients are calculated for each isotherm by the least squares method and are described analytically as

$$A = \sum_{i=0}^{5} a_i T^i \;;\; B = \sum_{i=0}^{6} b_i T^i \;;\; C = \sum_{i-0}^{6} c_i T^i \tag{2}$$

The equation (1-2) describes all the experimental data with an average error of 0.05-0.1%. The coefficients a_i, b_i and c_i have the concentration dependences. The generalization of the experimental data is of great interest in vein of information storage in the form of equation and prediction of properties of the object investigated. This method allows to predict the properties of the third solution with the help of the two ones and also to extrapolate the properties of the system.

The analysis of coefficients of the Eq. (1), depending on concentration, has allowed to offer the following equations, transferring concentration dependences for all investigated binary systems:

$$\rho = \sum_{i=0}^{5}\sum_{j=0}^{4} a_{ij}\, p^i (100-x)^j + \sum_{i=0}^{5}\sum_{j=0}^{4} b_{ij}\, p^i (100-x)^j \cdot T + \sum_{i=0}^{5}\sum_{j=0}^{4} c_{ij}\, p^i (100-x)^j \cdot T^2 . \tag{3}$$

Using the obtained values of coefficients a_{ij}, b_{ij} and c_{ij}, it is possible to define values of density of mixtures with satisfactory accuracy at high pressures, temperatures and different concentrations.

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Ab Initio CALCULATION OF THE TRANSPORT PROPERTIES OF HEAVY WATER IN THE DILUTE GAS LIMIT

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The dilute gas shear viscosity, self-diffusion coefficient, and thermal conductivity of heavy water (D_2O) were calculated at temperatures from 250 K to 2500 K employing a highly accurate *ab initio* pair potential and the kinetic theory of molecular gases [1-3]. The results [4], which have estimated uncertainties of (2–4)% (0.95 confidence level), significantly improve our knowledge as there are only few experimental data available for viscosity, no experimental data for the self-diffusion coefficient, and only data with large uncertainties for the thermal conductivity. The calculated transport property values will be used to develop the zero-density parts of new IAPWS reference correlations.

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THERMODYNAMIC CALCULATION AND 3D MODELING OF THE P-T-X DIAGRAM CU-PB-SE AND AG-PB-SE SYSTEMS

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Data for P-T-X diagrams of ternary chalcogenide systems is significantly less than T-X-Y phase diagrams for condensed state. In this work from the concepts thermodynamics of heterogeneous systems the equations for calculation of the partial pressures in the ternary system on the basis of thermodynamic functions of formation of compounds and liquidus coordinates were obtained. From the condition of equality of chemical potential components of AmBn in the equilibrium liquid and solid phases following relations was received:

$$\Delta G_T^{exs,l} = \Delta H_T^{0,s} - T(\Delta S_T^{0,s} + R\ln x_A^m x_B^n) \qquad (1)$$

where $\Delta G_T^{exs,l} = m\Delta\overline{G}_A^{exs,l} + n\Delta\overline{G}_B^{exs,l}$) ; $\Delta\overline{G}_A^{exs,l}$, $\Delta\overline{G}_B^{exs,l}$ - are the partial excess free energy of A and B in liquid solution, saturated by A_mB_n; $\Delta H_T^{0,s}, \Delta S_T^{0,s}$-are enthalpy and entropy formation of A_mB_n from liquid components; T, x_A, x_B- are temperature and mole fractions for liquidus. Based on the positions of the first degree homogeneous functions for calculation $\Delta\overline{G}_A^{exs,l}, \Delta\overline{G}_B^{exs,l}$ based on the values $\Delta G_T^{exs,l}$ in Eq (1) are obtained:

$$\Delta\overline{G}_A^{exs,l} = \left[\Delta G_T^{exs,l} + (1-x_A)(\partial G_T^{exs,l} / \partial x_A)\right] x_A / m$$

$$\Delta\overline{G}_B^{exs,l} = \left[\Delta G_T^{exs,l} + (1-x_B)(\partial G_T^{exs,l} / \partial x_B)\right] x_B / m$$

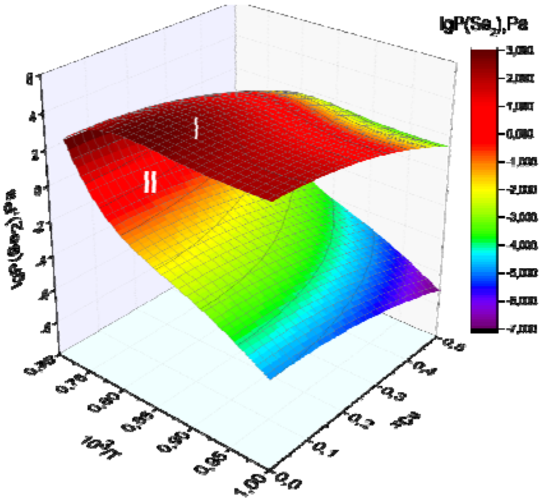

Fig. 1. 3D model of the P-T-x diagram for the partial pressure of Se_2 on the PbSe liquidus surface in the ternary Cu-Pb-Se system. 1- area PbSe-Se (ed.2); 2-area PbSe-Pb (ed.3).

From the known the thermodynamics relationships of solutions we have:

$$\ln p_i = \Delta G_i^{exs,l} / RT + \ln(x_i p_i^0) = \ln(x_i p_i^o \gamma_i),$$

where γ_i is thermodynamic activity coefficient. To approximate and 3D visualization of the information received for the liquidus surface AmBn compounds in the ternary system A-B-C, in particular PbSe (where *m*=*n*=1) compound in the system Me(Ag,Cu)-Pb-Se , the following equation has been used:

$$\ln p_{Se_2}(Me-Pb-Se) = f_{PbSe}(10^3/T) + \Delta\ln p_{Se_2} x_{Me}^n$$

The first term is an analytical expression of $\ln_{p_{Se_2}}$ on 10^3 / T along to curve of PbSe liquidus in the binary system Pb-Se, the second term takes into account the change $\ln_{p_{Se_2}}$ depending on the content of Cu and Ag. For the areas of liquidus PbSe-Se and PbSe-Pb for the Cu-Pb-Se syrtem the following relationships, respectively, were obtained:

$$\ln_{p_{Se_2}}\text{(Pa)}=[-1281+5624(1000/T)-9190(1000/T)^2+6648(1000/T)^3-1797(1000/T)^4]-10.35\,{x_{Cu}}^2 \qquad (2)$$

$$\ln_{p_{Se_2}}\text{(Pa)}=[2026-8778(1000/T)+14247(1000/T)^2-10259(1000/T)^3+2759(1000/T)^4]-8.36\,{x_{Cu}}^2 \qquad (3)$$

The calculations and 3D visualization of the P-T-x diagram for the partial pressure of Se_2 on the PbSe liquidus surface of the ternary Cu-Pb-Se and Ag-Pb-Se systems were performed by using OriginLab software.

Keywords: Thermodynamic, 3D modeling, P-T-X diagram.

THE STUDY OF OBTAINING OF CARBON NANOTUBES BASED ON C_5 FRACTION WITH CVD METHOD

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Chemical vapor deposition (CVD) is one of the perspective and economic viable methods for nanocarbon production. In this study, as a raw material, C_5 fraction boils at 30-70ºC were pyrolyzed in the CVD, between 10-30 min, at 750-900 ºC temperature in the argon atmosphere with using hydrogen gas as a reductive on this device. As the catalyst during the process ferrocene was used and as bearer MgO was utilized placed on iron with special method.

The experiments show that, synthesis of the nanocarbon without ferrocene catalyst is impossible and furthermore, the rate of gas mixture and time affect output and properties of the product: in case of H_2:Ar = 2:1 ratio at 850°C, the output of nanocarbon is 13.6%, but the result increased up to 17.4% by enhancing the amount of hydrogen gas to double in the system. The investigation the effect of time on process has shown that, the output value is 10.4% if the process takes 10 minutes, but when the time is up to 20 minutes, the amount of nanoparticles increase to 17.4%, during this time the diameter and height of nanoparticles increase linearly, high value of time from this point breakdown occurs between carbon bonds, as a result the amount of amorphous carbon particles rise. Analysis had been conducted with "TruSpec Micro" present that, the pyrolysis products consist of 97.2-99.0% carbon particles and 1.00-2.78% H. Structure and properties of nanocarbon were determined with using scanning electron microscope (SEM) and detected that at 850°C height and diameter of synthesized nano carbon particles are 65±5 nm and 27±4 nm respectively and it is formed carbon nano tubes directed to different directions.

So, investigations have shown that carrying out of coking process of catalytically treated C_5 fraction under optimum conditions it is possible to achieve the formation of nano carbon tubes. It is possible to control both the output and height of the carbon nano tubes and their properties with adjusting the temperature, time and the amount of gas supplied to the system during the process. Thus, the composition and properties of nano carbon allows using it for various purposes.

THE DETECTION OF *E. coli* USING LATERAL FLOW IMMMNOASSAY OF PEI MODIFIED Fe3O4/Au NANOPARTICLES

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Lateral flow immunoassay system is an effective way for identification of diagnostic, food analyzes and environmental. This microfluidic system provides easily commercial success, as known by sales of pregnancy kits [1,3]. Nowadays, paper based system has been using more efficiently due to its low cost, simple, easy, and user-friendliness, utilizing mostly for colorimetric and qualitative detection, but recently new technologies capable of obtaining quantitative researching such as conventional fluorescence, time resolved fluorescence, phosphorescence, Surface Enhancement Raman Spectroscopy have been demonstrated [4].

In This study, we report the preparation of iron nanoparticles, casein as a substrate, and main target *E. coli* with rennet enzyme including a bond cleavage to release bacteria. Substrate is covalently linked to iron particles and *E. coli* as a target bacterium to consist of magnetic particle based substrate conjugate as a sandwich model. When rennet enzyme cuthe casein conjugate to release bacteria from iron particles, the free *E. coli* was separated from intact casein conjugates by a magnetic field. Iron particle-casein-bacteria antibody were prepared as an enzyme substrate. Target bacteria into the solution was detected on the paper based test strips using SERS. The optimum concentration of the casein was determined on the test line using SERS with the aid of Raman label (DTNB).

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RESEARCH WORKING PROCESS OF A DIESEL ENGINE USING BUTANOL-CONTAINING FUELS

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The scientific contribution of the performed work consists in the development of new theoretical provisions for the justification of the working process of diesel engines in the application of alternative fuels. Theoretical and experimental studies of the working process of a diesel engine of dimension 100x125 mm on the ESC cycle and full load curve.

The influence of mixtures of diesel fuel with butanol on power, fuel and economic, ecological and dynamic indicators of the working process was analyzed. The working process parameters were determined, which ensure NOx emissions corresponding to the ecological level of Euro 5, and the minimum emissions of soot.

Combinations of the degree of recirculation of exhaust gases and cyclic fuel supply have been defined, which ensure a minimum emission of NOx for regimes of a 13-step test cycle while maintaining the diesel power ratings. An estimation of the efficiency of the combustion process on the indicator diagrams and the value of the indicator efficiency of the engine was made.

The results of the studies showed the effectiveness of using a mixture of diesel fuel with butanol, containing 15% butanol, as an alternative fuel for diesel engines. Compared with diesel fuel, specific consumption increases and engine power is reduced by no more than 2%, the indicator efficiency is increased by ~ 1.5%, emissions of soot are significantly reduced (up to 17%), nitrogen oxides are slightly reduced.

EXPERIMENTAL INVESTIGATION OF THE INFLUENCE OF THE NANOPARTICLES TiO_2 ADDITIVES ON THERMOPHYSICAL PROPERTIES OF R141b

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Recently, the information given in the literature on the influence of nanoparticles additives on the thermophysical properties of coolants and working substances of refrigerant systems as well as on the intensity of heat transfer processes very often disagree. To estimate the intensity of heat transfer processes in refrigeration systems, it is necessary to have information about the thermophysical properties of nanocoolants and nanorefrigerants.

In the presented study the model refrigerant R141b was chosen as the base liquid for the preparation of the nanofluid. TiO_2 nanoparticles with a size in the powder of less than 25 nm (CAS No. 1317-70-0, Sigma-Aldrich) was used as additives. To prepare the nanofluid a two-stage method was used. The mass fraction of nanoparticles in nanofluid was 0.1%. It was impossible to prepare a colloidally stable system of R141b / TiO_2 nanoparticles without surfactants. After preliminary researches, it was decided to use surfactant Span80 (CAS No. 1338-43-8, Sigma-Aldrich) in mass fraction 0.1 % for the preparation of nanofluid R141b / TiO_2 nanoparticles.

Measurements on the surface tension of the samples were carried out in the temperature range of 290-345 K. Expanded uncertainty of surface tension mesurement was 0.21 mN m^{-1} (0.95 level of confidence).The experimental apparatus implemented differential capillary rise method.

Viscosity measurements for the samples in the temperature range of 285-295 K were carried out using an experimental setup principally composed a glass capillary viscometer with a suspended level. Expanded uncertainty of measurements was 0.051 $mm^2\ s^{-1}$ (0.95 level of confidence). Viscosity measurements for the samples in the temperature range 295-355 K were carried out using an experimental setup based on the rolling-ball method. Expanded uncertainty of measurements was 0.6%.

The thermal conductivity measurements of the samples were carried out in the temperature range of 290-350 K by the transient hot wire method. Expanded uncertainty of measurements did not exceed 0.0017 $W \cdot m^{-1} \cdot K^{-1}$.

Measurements on the heat capacity of the samples were carried out in the temperature range of 290-345 K by an adiabatic calorimeter. Expanded uncertainty of measurements did not exceed 0.75%.

The effect of additives of nanoparticles and surfactants on surface tension and thermal conductivity was no considerable. The nanoparticles additives into R141b lead to viscosity increased by 0.8-1% and surfactant additives into R141b lead to significantly decreased in viscosity (by 3-4%). The nanoparticles additives into R141b lead to heat capacity decreased by 1.5-2%. Heat capacity increased insignificantly with surfactant additive.

The effects of nanoparticles TiO_2 and surfactant Span80 on the temperature dependence of the thermophysical properties of the refrigerant R141b are analyzed in detail in the report. We can state that the effect of nanoparticles and surfactants additives is ambiguous. It was shown the additivities rule could not use to calculate nanofluids heat capacity. It is shown the significant effect of nanopartickes additives on the viscosity of R141b based nanofluid. But there is an ability to regulate nanofluid viscosity by surfactant Span80 additives.

The availability of experimental data obtained under consistent and reproducible conditions creates many opportunities for the development of new models for predicting properties of nanofluids.

SYNTHESIS AND CHARACTERIZATION OF NI DOPED TIO$_2$ NANOPARTICLES AND INVESTIGATION OF THEIR PHOTOCATALYTIC ACTIVITY

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Namiq SHIKHALIYEV, Ilaha HASANOVA, Mirjavid AGHAYEV, Sarvinaz HAJIYEVA,
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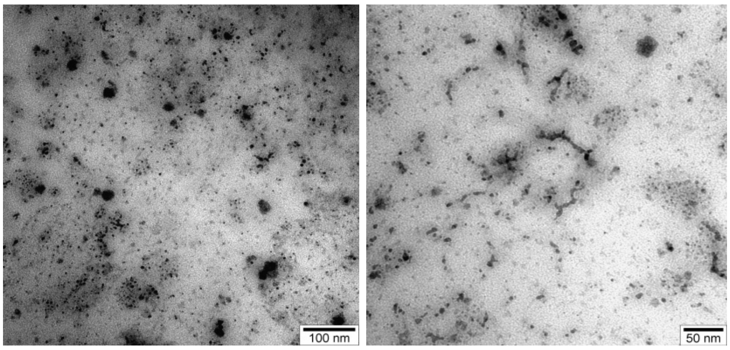
Photocatalytic technology has been applied widely in various fields such as environmental purification, water enviromental safety, the air and health quality in various environmental compartments, anti- bacterial uses and self-cleaning. Titanium dioxide is well known as harmless photocatalyst. Because of these photocatalytic properties, application of titanium dioxide spreads increasingly.

Different dopants are used in titanium dioxide for the absorption of visible light, such as transition metal ion doping (Fe, Co, Ni, Cu, Zn and Zr) has been found to be efficient dopants for improved photostability and bandgap tuning. In this work, we report synthesis and characterization of titanium dioxide nanoparticles doped with nickel. Nickel doped titanium dioxide nanoparticles were successfully synthesized by sol-gel method. X-ray diffraction (XRD), transmission electron microscopy (TEM), FT-IR and UV–vis spectroscopy techniques were used to characterize the samples.



The doped TiO$_2$ nanoparticles in general showed higher photocatalytic activities than the pure ones. Photocatalytic activities of samples for acetamiprid degradation were investigated and the Ni-doped titanium dioxide samples showed higher photocatalytic activity than undoped titanium dioxide.

SYNTHESIS OF GRAPHENE OXIDE MODIFIED SUPRAMOLECULAR ENSEMBLES AND THEIR APPLICATION

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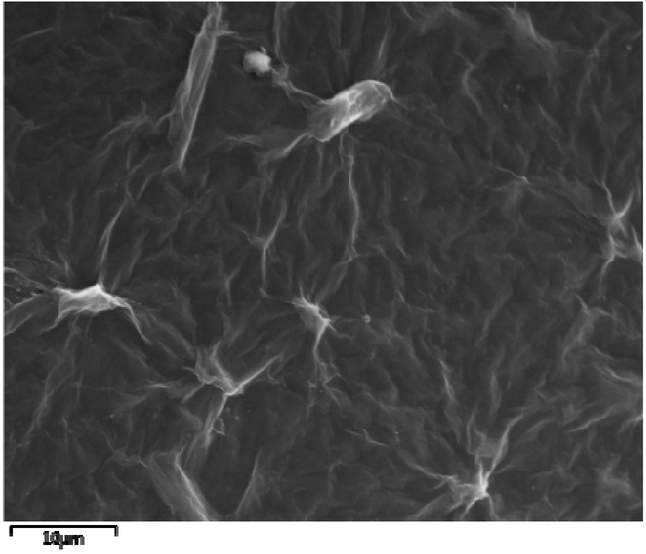
Graphene oxide (GO) is a single-atomic layered material with oxygen-containing groups, made by the powerful oxidation of graphite, which is cheap and abundant. One of the advantages of the GO is its easy dispersability in water and other organic solvents, as well as in different matrixes, due to the presence of the oxygen functionalities.

Functionalization of GO can fundamentally change GO’s properties. The resulting chemically modified graphenes could then potentially become much more adaptable for a lot of applications, for example in optoelectronics, biodevices, as a drug-delivery material and so on.

In this paper we report about synthesis of ensembles on the basis of GO nanolayers with vanadium oxide and spiderweb of Avicularia versicolor. The structure and morphology of synthesized ensembles were studied with TEM, XRD, FTIR, AFM methods.

a) SEM image of GO nanolayers



b) SEM image of VO_2 nanoparticles

The ensemble on the basis of graphene oxide and vanadium oxide was used in battery for decreasing it’s heating. Obtained results demonstrate decreasing heating up to 1.5%. The ensemble on the basis of graphene oxide and spiderweb was used in concrete to increase its solidity. It was found that this ensemble increase solidity of the concrete up to 2%.

ELECTRICAL PROPERTIES OF CdMnTe EPTAXIAL FILMS IRRADIATED BY GAMMA QUANTA

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It has been studied impact of γ-irradiation on electrophysical and photoelectrical properties of Cd1-xMnxTe (x=0.07) epitaxial films depending on γ-irradiation dose.

Epitaxial films were obtained on glass substrate in a vacuum (1÷2)10^{-4}Pa by Molecular Beams Condensation method. It was determined the optimal conditions (T_s=1000-1100 K, T_{sub} = 570-670 K) to obtain epitaxial films with perfect structure and a clean, smooth surface, without the inclusion of the second phase by using of additional source of Te vapor and temperature control.

VAC of initial and γ-irradiated samples of $Cd_{1-x}Mn_xTe$ (x=0.07) epitaxial films, with thickness d=15μm on glass substrates has been studied. In the initial samples of $Cd_{1-x}Mn_xTe$ in VAC there is observed a linear part $J \sim U$ corresponding to Ohm's law and quadratic part $J \sim U^2$. Further, samples were irradiated by γ-quanta at doses D_γ≤23kGy.

Analysis of the curves can be carried out within the framework of theory of injection currents in solid solutions with no-activation conductivity. The observed character shows that within the irradiation of $Cd_{1-x}Mn_xTe$ films with small doses D_γ=100Gy, a number of deep levels are formed in the forbidden band in which electrons take part, and it leads to a decrease in conductivity. Further irradiation D_γ =400Gy leads to an increase in the conductivity, resulting in the appearance of an impoverished quadratic region. With a further increase in the irradiation dose D_γ=1.5kGy, the current decreases, and trapped quadratic region is again observed, but in the dose D_γ=3kGy the current again increases, irradiation up to doses D_γ=25kGy leads to decreasing of conductivity.

The effect of γ-radiation on the photoconductivity of $Cd_{1-x}Mn_xTe$ (x=0.07) epitaxial films was studied. In the initial samples of $Cd_{1-x}Mn_xTe$ epitaxial films there is a wide band in the photoconductivity spectrum, the spectral range covers the wavelength region λ=370nm-1700nm. The band gap, calculated from the photoconductivity spectra (λ=765nm), is equal to E_g=1,62eV which corresponds to our theoretical results.

The significant changes in the VAC and the photoconductivity of $Cd_{1-x}Mn_xTe$ epitaxial films after irradiation by γ-quanta at doses D_γ ≤25kGy make it possible to create detectors of ionizing radiation on their basis.

This work was supported by the Science and Technology Center in Ukraine, Grant № 6288.

RHOMBIC POLYHEDRA OF PROPELLANIC NATURE FOR THERMODYNAMIC STUDIES

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Radial rhombic polyhedra with propellanic characteristics can be obtained by repeating the following operation: the two vertices lying opposite diagonal of each rhomb of an all rhomb covered structure (zero-generation, Rh_0) are joined by a point. New vertices opposite to the parent vertices are added. The previously obtained points and those lying in the proximity of each parent vertex are merged, forming multi-shell rhombohedral clusters. Because the two diagonals are not identical topologically, each generation consist of two isomers [1,2]. Those isomers can be further thermodynamically investigated by means of Gibbs free energy using Gaussian 09w and GaussView 5.0.

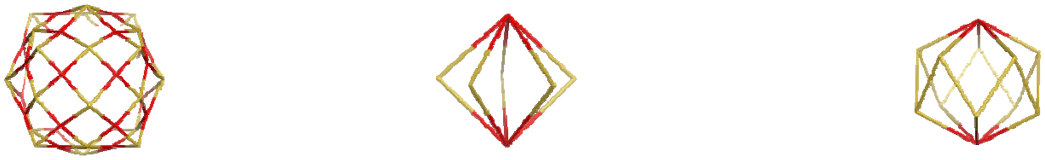
C_5H_6 = [1,1,1] Propellane

$Rh_{2.3}.5 = K_{2.3}$

C = $Rh_{2(3.3)}.8$ and ppl points (in red)

Cube first generation rhombic structure, ppl^{1}C ($Rh_{2(4.4.4)}.14$ envelope)

Figure 1. Propellane, $Rh_{2.3}$ and propellation from cube starting



$Rh_{2(4.8.8.8.8.8.4)}.50$

$K_{2.5} = Rh_{2.5}.7$

$Rh_{2(5.5)}.12$

Figure 2. Some rhombic structures

Keywords: multi-shell clusters, operation on map, quasicrystals, non-connected vertices, m-partite graphs

Acknowledgement
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ZINK PHENOLATES - NEW HIGHLY ACTIVE CATALYSTS IN THE CYCLOADDITION REACTION OF CARBON DIOXIDE AND ETHYLENE OXIDE

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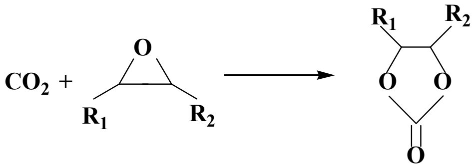
The chemical utilization of CO_2 is an important topic. One of the more successful processes for CO_2 utilization for material synthesis is the catalytic production of cyclic carbonates from epoxides. Incorporation of CO_2 into carbonates is a potentially significant transformation for the decrease of carbon dioxide level in the atmosphere.

Many new methodologies for cyclic carbonate synthesis from CO_2/epoxide coupling have been developed. The two most active catalyst families are based on the series of bis(salicylaldiminato)metal complexes and tetradentate metal complexes. Catalysis based on (salen)metal complexes have seen significant progress. Salen-metal catalysts originally evolved from the metal porphyrinate catalysts. They have measured one of the highest TOFs for homogeneous metal-based catalysts. In particular, a TOF of 100-500 mol AK/mol Cat•hour was observed.



The recent challenges in cyclic carbonate synthesis have focused on limiting the use of inorganic catalysts or replacing them with new, environmentally benign free metal media in a view to develop green chemical synthesis.

In the present work, the coupling reactions of carbon dioxide with epoxides to produce five-membered cyclic carbonates (ethylene, propylene, 1-hexene, cyclohexene, styrene, etc, carbonates) were efficiently catalysed by Zn-phenolates. These catalytic systems were found to be efficient catalysts without any co-catalyst for the coupling reactions of CO_2 with neat epoxides. At conditions: P_{CO2}=1,0-10,0 MPa; T=20-120°C; τ=30-120 min and the concentration of Zn-phenolate [Zn]= $0{,}5\cdot10^{-3}$-$1{,}0\cdot10^{-3}$ mol/L the activity and productivity of these catalysts were: 92-99% of conversion (with stereoselectivity of 95-99%) and TOF= 600-3000 mol AK/mol Cat•hour.

The Zn-phenolate catalytic systems were also applicable to other terminal epoxides with good yield of cyclic carbonates. The work reported has the potential to improve the catalytic efficiency and reduce cost of products for larger applications.

SORPTION OF U(IV) ONTO AMIDOXIMATED POLY[*N*-(3,4-DICYANOPHENYL)ACRILAMIDE]

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Uranium is one of the most dangerous heavy metals in the environment because of its chemical toxicity and radioactivity. Excessive amounts of uranium have entered into the environment through the activities associated with the nuclear industry [1]. Uranium is usually found in the environment in the hexavalent form. The general methods developed for the recovery or removal of uranium ions from aqueous solutions are extraction, precipitation, ion exchange and sorption. Among those approaches, sorption is commonly used for the recovery of uranium ions because of its high efficiency, ease of handling, and the availability of different adsorbents [2].

The amidoxime adsorbents for the recovery of uranium from aqueous solutions were development in the late 1970s and early 1980s. Amidoxime polymers were prepared by synthesizing and then amidoximating polymers containing amidoxime precursor cyano groups [3].

The aims of this study are to investigate the influence of various experimental parameters on uranium adsorption by amidoximated poly[*N*-(3,4-dicyanophenyl) acrilamide] and to evaluate the adsorption process in terms of equilibrium, kinetics and thermodynamics conditions.

Adsorption experiments of uranium ions on amidoximated polymer were carried out by using batch method. The effects of contact time, pH, initial concentration, and temperature on U(VI) adsorption by amidoximated polymer were investigated. For each parameter, after the adsorption, the final concentration of uranium in the solution was determined in the UV-Vis spectrophotometer at 650 nm using the Arsenazo(III) complex method.

For the kinetic conditions, results were applied pseudo-first order and pseudo-second order kinetic models. The results showed that the adsorption kinetic behavior of U(VI) on amidoximated polymer fitted to the pseudo-second order kinetic. For the equilibrium conditions, the equilibrium data in aqueous solutions were applied to different sorption isotherms such as Freundlich, Dubinin-Radushkevich, Temkin and Langmuir. The adsorption equilibrium data fitted very well to Langmuir model for U(VI) adsorption by amidoximated polymer. For the thermodynamic conditions, the thermodynamic parameters, ΔH^o, ΔS^o and ΔG^o, were calculated and evaluated. The negative value of ΔG^o (-2.92 kJ/mol) indicates the spontaneity and the positive value of ΔH^o (15.14 J/mol) shows the endothermic nature of the adsorption process for U(VI) adsorption by amidoximated polymer.

The present study was supported by Van Yuzuncu Yil University Scientific Research Projects Support Unit (Project number: 2015-FBE-D031)

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ABOUT NEW APPROACH TO THE SOLUTION OF PROBLEMS OF LOW-PARAMETRICAL EQUATIONS OF STATE

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To the famous equation of state (ES) of Van der Waals which became an ancestor low-parametric the ES, in 2018 it is executed 145 years. Many hundreds of his empirical modifications, both private forms, and the generalized cubic equations for this time are offered, but the problem of receiving and choice of optimal ES is not solved. For evaluation test of the ES the results of calculations are compared to experimental data or with results of calculations for others known the ES. "Having proved" advantages of new ES, authors do not concern the reasons for which this optimization takes place. The reasons are, apparently, on a molecular scale. It is also apparent that the solution of this question will define the direction of works on creation of physically reasonable simple ES. Let's remind that loose coupling (practically its total absence) of ES of vdw-type with micro level is considered their main shortcoming. At same time, according to the main idea of systems approach, upon transition on the language of models, the same communications have to remain which were in reality. Therefore the ES as the model of a thermodynamic level, the model of properties - has to be a manifestation of properties of the molecular model which is its cornerstone.

Ideally, all parameters of models of two levels have to make sense and to be the obviously bound. As for low-parametrical, of a vdv-type ES, for them already "cognitive" requirements – about the sense of all parameters - are not fulfilled. Usually, authors of modifications assume that two parameters of new ES are make the same sense, as in the ES of Van der Waals. At same time, the sense of the others is not discussed at all. (Though the question of whether the sense of two parameters remains the same if new are added to the model, is not so simple). From here follows, that authors first shift responsibility for physics of the models on Van der Waals; secondly, that indeterminacy of the third parameter deprives of sense all ratios where it enters and as a result to the ES many questions appear; and, thirdly, that the solution of "a problem of the third parameter" obviously was restrained by the scientific authority of the Nobel laureate, of the creator well-known the ES.Questions to the ES of vdw-type were formulated by us repeatedly (see our works on the website www.csmos.ru). Let's emphasize only that at routine approach it is not possible to receive answers. For the solution of questions, it is necessary to eliminate the main defect of the equations, i.e. to connect them with a molecular scale. This problem managed to be solved within new molecular and thermodynamic model – the ES, based on the simple molecular model of the interacting point centers (IPC). Two of three deposits of new ES – configuration, all three parameters have the sense determined by manifestation of attractive and repulsions forces. The ES, received in assumption of hard repulsion of the centers, was generalized by the introduction of padding parameter considering its more realistic character..The operating parameters of two levels are introduced for the first time. Many the ES of vdw-type was included in a framework of new model. It transfers them to family of physically reasonable ES and allows to answer many questions. Such solution of the problem completely corresponds to application of a method of logical abduction and proves adequacy of the new model IPC.

EXPLORING CEPHALOSPORINS THROUGH QSAR AND MOLECULAR DOCKING

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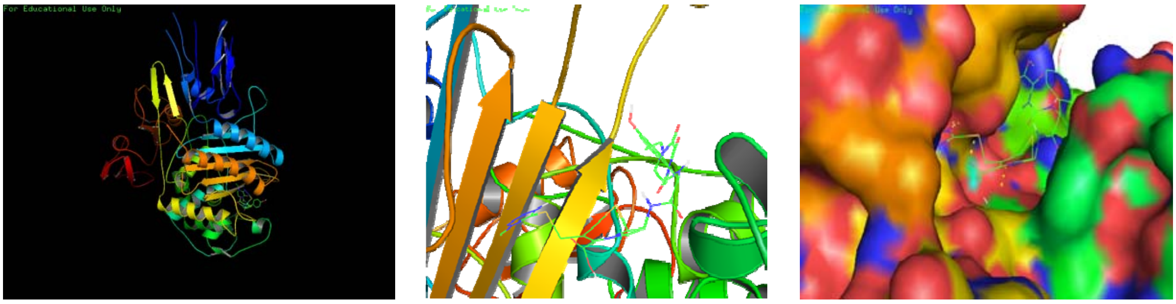
Discovered in 1945, cephalosporins represent an intensively studied class of β-lactam antibiotics used in the prophylaxis and treatment of infections with G+/- bacteria. They have the same action mode as penicillins by interacting with specific membrane proteins, penicillin-binding protein PBP, (not present in humans), preventing the cross-linking of the glycan polymer in the cell wall structure.

We present the results of our 31 ligands (currently used drugs) molecular docking [1] on 12 receptors, proteins belonging to G + and G- bacteria. Through QSAR algorithm based on Hypermolecule [2,3] concept we obtained a molecular descriptor that reflects the partial charges of each ligand [4]. We found the mathematical relationship between structure (Sum Descriptor= molecular descriptor) and biological activity (BA= Binding Affinity) BA=*f* ($SD_{charges}$) on each receptor. Statistically, ligands set-receptors interaction is better explained for *Neisseria gonorrhoeae* and *Actinomadura R39,* comparative with *Mycobacterium tuberculosis PonA1 or Staphylococcus aureus.*



Typical Figure. Cefoperazone, the best docked ligand, in glove-like binding site of 1QMF protein

Keywords: penicillin-binding protein PBP, transpeptidase domain TD, Binding Affinity BA, molecular docking, MLR, Hypermolecule, statistical parameters.

Acknowledgement

This work was supported by a grant of the Romanian National Authority for Scientific Research and Innovation, CCCDI—UEFISCDI, project number 8/2015, acronym GEMNS (under the frame of the ERA-NET EuroNanoMed II European Innovative Research and Technological Development Projects in Nanomedicine).

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EFFECTIVE INHIBITORS OF CORROSION ON THE BASIS OF HALOGOGENOUS COMPLEXES OF NATURAL OIL ACIDS

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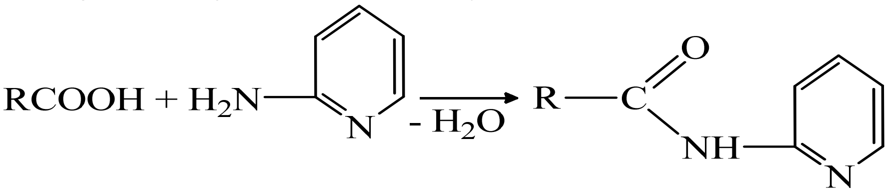
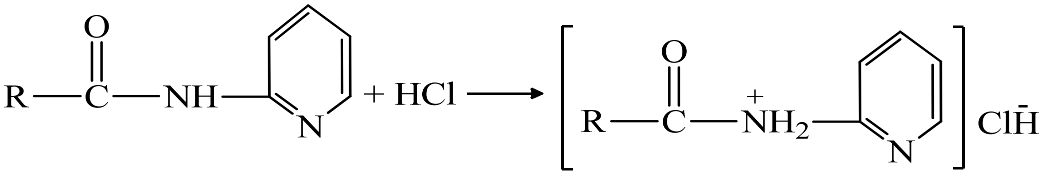
At the moment, the corrosion problem is one of the most serious problems in industrialized countries. This problem is even more serious in the petroleum and gas industry. Thus, more watering of the layers, increasing the amount and aggressiveness of water accelerates corrosion processes. One of the best ways to prevent corrosion processes is the use of inhibitors.

We have synthesized amide based on natural petroleum acids (NPA) separated from the kerosene fraction obtained from the processing of Azerbaijani oils and 2-aminopyridine:



Then the complexes were synthesized on the basis of the synthesized amide:



20 % solution of obtained amidine and complexes were prepared in the isopropyl alcohol and in 70 % solutions of the isopropyl alcohol in water. The effect of the prepared solutions on the kinetics of CO2 corrosion has been studied. The results are given in Fig 1 and 2.

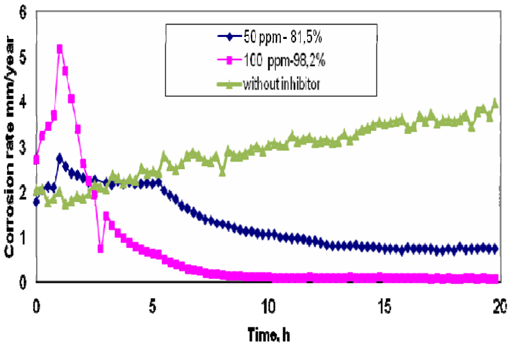


Fig.1. The inhibitory effect of NPA on CO2 corrosion of 20% solution in IPS of 2-aminopyridine and amide with complex of choloride acid

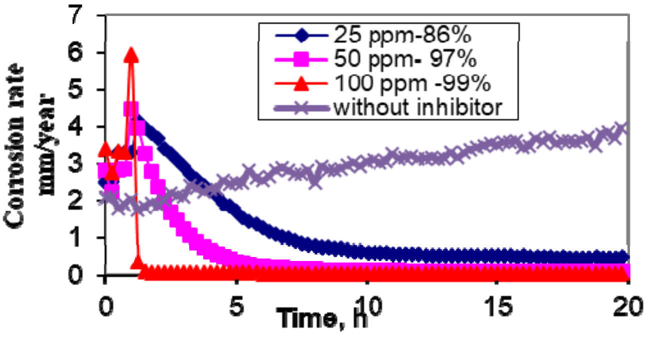


Fig 2. The inhibitory effect of NPA on CO2 corrosion of 20% solution in IPS of amide of aminopyridine

As shown in Fig. 1 and 2, the amidine chloride complex has a stronger effect than amide itself. Thus, the protection of the chloride complex against CO2 corrosion was 81.5 and 98.2% at 50 and 100 mg/l concentrations.

THERMOPHYSICAL PROPERTIES OF 1-BUTANOL AND DIESEL FUEL BLENDS

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Using of traditional diesel fuel in engine is increasing as the result of increasing of modern injection technologies. At results of these procedures, various environmental problems also increase. Environmental degradation of traditional fuels and using of various additives and renewable alternatives in internal combustion is main focus of research investigations in this field. 1-butanol has been proposed as an alternative to conventional gasoline, diesel fuels and using of them dramatically increased during the last years. From another side, current fuel injection systems of compression-diesel engines reach pressures up to 200 MPa for transport systems. Number of injections at such high pressures per cycle is expanding, the time of one injection process can be reduced and it is wished for to have exact control of injection rate shaping. That is why it is so important to have reliable knowledge of thermophysical properties of the fuel under high pressures, such as density, vapor pressure, viscosity, speed of sound, heat capacity etc. would allow modelling, understanding, and optimizing the processes in an internal combustion engine.

The (p,ρ,T) properties at T = (263.15 to 468.15) K, pressures up to p = 200 MPa, vapor pressure at T = (274.15 to 468.15) K, heat capacity at T = (253.15 to 468.15) K and ambient and saturated pressures were measured experimentally. An equation of state for fitting of the (p,ρ,T) data of 1-butanol + diesel mixture has been developed as a function of pressure, temperature and concentration. The thermophysical properties of 1-butanol and diesel fuel blends were calculated at high state parameters. The excess molar volumes V_m^E of 1-butanol + diesel mixture were calculated using the experimental values of investigated solutions. The molecular mass of diesel, which is necessary for these calculations, was used as the recommendations of various literatures.

THERMOPHYSICAL PROPERTIES OF 1-BUTYL-3-METHYLIMIDAZOLIUM TETRAFLUOROBORATE

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The first room temperature ionic liquid (IL), at the beginning of the twentieth century, the growing interest of ILs and scientific investigations have only begun since the 1980s. Investigations and practical applications of ILs during the last two – three decades have tremendously increased along with the results of their various excellent properties (negligible vapor pressure, large liquidus range, high thermal stability, high ionic conductivity, large electrochemical window, ability to solvate compounds of widely varying polarity, and etc.). In this case, thermophysical properties are very important during the analysis and application of ILs. The most important of those are density, viscosity, speed of sound, heat capacity *etc.*, from which more parameters can easily be derived, as shown in this paper.

In this work, investigations on [BMIM][BF_4] were done at temperatures from T = (273.15 to 413.15) K and from ambient pressures up to p =140 MPa. The objective is to substantiate and also to expand the thermophysical properties existing. Density ρ was measured using an Anton-Paar DMA HPM vibration-tube densimeter in the high-pressure region and an Anton-Paar DSA 5000 M model at ambient pressure, respectively, with an estimated experimental relative combined standard uncertainty of $\Delta\rho / \rho = \pm$ (0.01 to 0.08) %. The results were compared with the published literature values and an empirical multiparameter equation of state which covers the high-pressure region as well was established.

Additionally, the specific heat capacity at constant pressure c_p of [BMIM][BF_4] at temperatures T = (273.15 to 413.15) K and at ambient pressure were measured using the differential scanning calorimeter Pyris 1 DSC [6] with an experimental relative combined standard uncertainty of $\Delta c_p / c_p = \pm$ 0.5 %. Using these data, other thermophysical properties, like specific heat capacities at constant volume c_V, speed of sound u, and isentropic exponent κ_s at temperatures T = (273.15 to 413.15) K and pressures p up to 140 MPa were calculated.

The density values $\rho(p_0,T)$/kg·m^{-3} at ambient pressure and at temperatures T = (273.15 to 413.15) K are investigated using the Anton Paar DMA 5000M, DSA 5000M and DMA HPM vibration tube densimeters with an uncertainty of $\Delta\rho = \pm$ ($5\cdot10^{-3}$ to $3\cdot10^{-1}$) kg·m^{-3}. These values are necessary to check the accuracy of the investigated high pressure – high temperature (p,ρ,T) data using the small extrapolation of them to p= 0.101 MPa.

The speed of sound values $u(p_0,T)$/m·s^{-1} at ambient pressure and temperatures at T = (278.15 to 343.15) K are investigated using the Anton Paar DSA 5000M vibration tube densimeter and sound velocity meter with intervals of ΔT= (5-10) K and an uncertainty of $\Delta u = \pm$ 0.1 m·s^{-1}. These high accuracy values are necessary to check the accuracy of calculated speed of sound values u/m·s^{-1} at p= 0.101 MPa.

THERMAL CONDUCTIVITY OF BiNARY AND MIXED AQUEOUS ELECTROLYTIC SOLUTIONS

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Using an absolute method of coaxial cylinders, the thermal conductivity for binary and mixed aqueous solutions of alkali metal halides and lanthanide salts has been measured in the wide range of concentration, temperature and pressure. The standard uncertainty of measurements is ± 1.3%. The studied mixed salts did not chemically interact and did not form complex compounds in aqueous solutions.

The obtained experimental data for thermal conductivity of solutions have been compared with the values, calculated by using the methods of concentration dependences determination for thermal conductivity of solutions at $T = 25^{o}C$.

The numerical values for contributions of the dissolved salts cations and anions for the thermal conductivity of solutions have been determined for binary aqueous solutions of alkali metal halides using the concepts of «hydration and corrected radii of ions».

The concept of «isopiestic solutions consisted of water and two electrolytes with specified concentration and a common ion» was used as the basis for the developed technique of calculations for the mixed solutions thermal conductivity. It is shown that the thermal conductivity of the mixed solutions is an additive function for the appropriate values of thermal conductivity of the initial binary solutions that correspond to the figurative points with the same water activity and relative fractions of binary solutions forming a mixed solution.

It was found out that thermal conductivity for some of the mixed solutions of alkali metal halides at certain concentrations of the initial binary aqueous solutions is equal to thermal conductivity of water, i.e. the phenomenon «isothermal conductivity» takes place. For mixed aqueous solutions of lanthanides, this phenomenon is not observed.

A similar conception was proposed in the projected procedure for the thermal conductivity calculation of mixed aqueous solutions for three salts with specified concentration and the same ions. The Gibbs triangle is used for location of the figurative points of solutions for three salts, having the same water activity.

It is also shown that comparison of the thermal conductivity experimental data with the calculated values for mixed and ternary aqueous solutions found out by using the concept of «isopiestic solutions and additive effect of the individual cations and anions on the conductivity of solutions» have been conformed within ± 1.0 percent.

HETEROGENIZED BIFUNCTIONAL COBALT-CONTAINING CATALYTIC DITHIOSYSTEMS FOR GAS PHASE AND SLURRY POLYMERISATION OF DIENES

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The bifunctional nickel and cobalt-containing catalyst-stabilizers, developed in IPCP of ANAS, have more attention because of their higher catalytic activities in dienes polymerization and polymer stabilization effect after process. However, as other homogeneous catalysts, these catalysts have disadvantages such as a short life time of active sites and difficulty of catalyst separation from received product. To pass these challenges and develop suitable systems for most of the industrial processes (slurry or gas-phase reactors), the immobilization of such catalysts is required. A gas phase process is lower in cost and energy consumption in comparison with a solution process, the homogeneous catalysts for dienes polymerization also must be heterogenized on a support to be applied in those processes. In addition, the heterogenization of the polymerization catalysts is necessary to avoid reactor fouling with finely dispersed polymer particles, to prevent excessive swelling of polymers, and to produce polymer particles of a desired regular morphology. Various inorganic materials, such as zeolites, silica gel, $MgCl_2$, Al_2O_3, MgO, etc, have been used as support to immobilize homogeneous polydienes catalysts. Nanomaterials [nanoclays, such as nanomontmorillonite (NMM) and nanohylloysite (NHS)] are more attractive candidates as support to immobilize homogeneous dienes polymerization catalysts. Nanomaterials have a large surface area and have exceptional physical and chemical properties, like small size, electron mobility, relatively high temperature, oxidation, basic and acid stability, making them useful support material for heterogeneous catalysis. For those reasons, the presence of nano support material can be expected to increase the catalytic activity, enhance the catalytic life time, and reduce the reaction time. Considering these advantages, nanomaterial immobilezed cobalt dithioderivatives+aluminumorganic compound (Co-DTD+AOC) catalytic dithiosystems have been prepared. Heterogenized on NMM and NHS bifunctional cobalt containing dithiosystems in the conditions: cobalt concentration on support- 0.030-0.072%; Al:Co=100:1; pressure of butadiene-0,1-2,5 MPa; temperature 20-80°C; reaction time 45-120 min, allow to receive 1,4-cis polybutadiene by the yield of 95.0-99.0; productivity of catalyst - 5000.0-10000.0 kg PM/g Co•hour; 1,4-cis-content– 93.0-98.0%; molecular mass- 25000-500000 and MMD - 1.8-2.5.

Received polybutadienes have been used to make rubber and tyre products.

THERMODYNAMIC ASSESSEMENT OF THE NOVEL GENERATION OF SYNTHETIC WORKING FLUIDS FOR REFRIGERATION SYSTEMS, HEAT PUMPING AND POWER GENERATION

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By reducing the use and emissions of halogenated chlorofluorocarbons (CFCs) and halons the Montreal Protocol designed 30 years ago in September 1987 confirmed that global ozone depletion could be attributed to atmospheric chlorine. The use of production of CFCs was effectively prohibited after January 1, 1996. Different industries turned to HCFCs as substitutes for CFCs but they also have become subject to scheduled phase out by 2020. The leading candidates for the major use of CFCs and HCFC-22 are hydrofluorocarbons (HFCs). The HFCs posses zero ozone depletion potential (ODP) but the significant global warming impact (GWP). The Kigali agreement (2016) developing the Paris Climate Agreement (2015) will phase down HCFs over the next 20 years, preventing as much as half a degree Celsius of additional warming.

As alternatives for HFCs (R134a, R404A, R410A, et al.) as high GWP fluids replacement the hydrofluoroolefins (HFOs) have been proposed. The HFOs refrigerants have ODP value of zero, a very small value GWP, low toxicity and mild flammability but the optimal choice of HFOs depends on study of thermodynamic and thermophysical properties. In this work fundamental equations of state, data for the critical parameters, thermodynamic properties along the saturation curve and single phase region, transport properties, surface tension, speed of sound for R1234ze(Z), R1234yf, R1234ze(E) as working fluids are considered to evaluate the thermodynamic performance of new HFO-refrigerants.

THERMAL CONDUCTIVITY MEASUREMENTS OF REFRIGERANTS R32, R134a AND THEIR MIXTURES AT ZERO DENSITY

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Refrigerants are very important for many of the social demographic and technological applications and advancements that have occurred in developing and developed countries. The modern tendency is to use blends to optimize the characteristics for the industrial applications. The idea is to blend R32 (difluoromethane) with a sufficient amount of the nonflammable R134a (tetrafuoroethane) to go below the limit of flammability and to use the excellent thermodynamic efficiency of R134a. This paper presents the thermal conductivities measurements of the HFC-R134a, HFC-32 and their binary mixtures in the dilute gas state at temperatures from 292.36 to 365.05 K. The investigation was carried out by vertical coaxial cylindrical stationary method. The fluid surrounds the cell and fills the gap between two vertical cylinders. The compositions of the binary mixtures were 26.2 mas % of HFC-32 and 51.4 mas % of HFC-134a. The accuracy of the measurements was assessed by measuring the thermal conductivity of a primary standard toluene, refrigerant R22 and helium. The deviations of our results with the results of other workers for HFC-32 and HFC-134a do not exceed a maximum deviation of less than ±2.5 %.

To interprete the behavior of experimental results for the thermal conductivity of gaseous mixtures at low pressure a variation of the Lindsay–Bromley relation based on the Wassilieva–type equation have been developed for calculation in mixtures with large differences in molecular size.

FORMULATION FOR HFO-REFRIGERANTS TRANSPORT PROPERTIES OF 2,3,3,3-TETRAFLUOROPROPEN AND ZIS-1,3,3,3-TETRAFLUOROPROPENE IN THE RARIFIED GAS STATE

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In the last years the HFO-substances are selected as excellent working fluids for refrigeration. This paper is a continuation of study of the properties of HFO-class refrigerants and is intended to fill the limited amount of transport properties information on HFO-refrigerants and also provide reliable methods for their prediction in the dilute gas thermodynamic state. The scheme is based upon the combination of strongly theoretical approaches and heuristic scenarios. It is shown that the fundamental theoretical models allows the evaluation of the transport properties of pure 2,3,3,3-tetrafluoropropene and zis-1,3,3,3-tetrafluoropropene.

The low-pressure thermal conductivity was been represented by Mason–Monchick and Chapman–Enskog equations in terms of the collision integrals derived from the kinetic theory of dilute gases. The results were used to examine the behavior of the Maxwell factor. Thermal conductivity, diffusion coefficient and viscosity data for the rarified gas state are presented.

THERMOPHYSICAL PROPERTIES OF SEAWATER SAMPLES

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Water covers a major fraction of Earth's surface, and also part of about 97% of seawater. The changing of changing of temperature in atmosphere, melting of ice etc. change also seawater quality and properties. The thermophysical properties also are changing. The changing of climate and increasing of middle temperature in the Earth and Seawater surface, aslo speeding up evaporation of seawater.

In this case, we analysed the seawater samples from various parts of world: Atlantic Ocean, Pasific Ocean, Baltic Sea, Black Sea, Caspian Sea, Dead Sea, Mediterranean Sea, Red Sea etc. were studied. As deep of Ocean or sea increases, density also decreases. As temperature increases, density mostly decreases. As salinity of the seawater increases, density also increases. The density of seawater also changes in dependence on the depth below the sea surface due to the static pressure. In this case, the measurements were carried out at various temperatures, salinities and high pressures.

The density measurements at the high pressures were carried out using the Anton-Paar DMA HPM vibration-tube densimeter. The density measurements at ambient pressure also were carried out using the Anton-Paar DMA 5000M densimeter. The viscosity of samples were analysed using the SVM3000 Stabinger Viscometer. The chemical analysis of samples (cations and anions) were analysed using the IRIS Intrepid II Optical Emission Spectrometer and DX 100 ion chromotography.

An empiric equation of state for fitting of the (p,ρ,T) data of the seawater samples has been developed as a function of pressure, temperature and salinity of water. This equation is used for the calculation of the thermophysical properties of samples.

CALCULATION OF PHASE EQUILIBRIA OF SALT HYDRATES FOR PREDICTING THEIR BEHAVIOR AS PHASE CHANGE MATERIALS

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Phase change materials (PCM) can be used as latent heat thermal energy storage (LHTES) to reduce load fluctuations and improve the efficiency of heating and cooling systems in buildings, of industrial processes, and power plants. By the use of solid-liquid phase transitions, PCM’s deliver high heat storage densities at small and precise temperature ranges. Tailoring the melting temperature of the employed compound to the specific application temperature would yield the most optimal efficiency gain. Since the availability of pure substances with suitable melting temperatures is limited, eutectic mixtures of different compounds have been of high interest. More specifically, eutectic mixtures of salt hydrates are being studied as a suitable PCM´s for low and high temperature applications as a cost-effective solution.

In this work, framed within the PCM Screening project, the objective is to predict and analyze the behavior of well-known and unexplored salt hydrates at solid-liquid equilibrium to determine the melting properties at different hydration levels and assess their suitability for any specific application and working temperature.

The methodology consists in the gathering and analysis of existing empirical and semi-empirical thermodynamic data, especially heat capacities and properties of formation, to derive a suitable Gibbs’ free energy model for the solid composition, while an excess Gibbs’ free energy model is assembled for the liquid solution. Both models must be integrated to find the liquid-solid equilibrium of the salt hydrates of interest.

First calculations for the phase equilibrium of magnesium sulphate (MgSO4) and water will be shown by combining semi-empirical thermodynamic data of different hydrate levels and a suitable ion interaction Pitzer model for the liquid solution. The results are then compared to experimental phase equilibria curves to prove the appropriateness of the model and its future perspectives.

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EXPERIMENTAL STUDY ON THE FERROFLUID FLOW IN A MINI-SIZED CHANNEL

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Ferrofluids are colloidal mixtures comprising of ferromagnetic nanoparticles and a carrier fluid. These fluids are specific materials with their excellent magnetic properties and they can be manipulated by applying an external magnetic field. This provides them a contactless actuation. So that, they can be used for many different potential application areas such as cooling of electronic devices, drug delivery, energy systems etc. Along with the developing technology, it has become a necessity to reduce the size of electronic and mechanical devices and to increase the system efficiency. Therefore, recently mini pump systems are drawing quite attention of the researchers.

In this study, it is aimed to manipulate the ferrofluid sample in a mini sized channel with a square cross section by the effect of the magnetic field generated by the permanent magnets placed on rotors. The system contains two rotors, two step motors, a square cross-section mini channel, eight magnets and a microcontroller. The experiments were conducted for different motor frequency values. In the previous study [1], similar system was considered and the maximum flow rate of 30µl/min was obtained. In order to increase this flow rate value some parameters have been improved in the present study such as location of permanent magnets, rotor dimensions and channel module geometry. The results indicated that the flow rate values increase with the improved system design. Moreover, it is observed that the flow rate generated varies with different frequency values.

Keywords: Ferrofluid, mini channel, magnetic field, permanent magnet.

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MOLECULAR STRUCTURE AND VIBRATIONAL SPECTROSCOPIC STUDIES ON 3-((2-ISOPROPYL-5-METHYLPHENOXY)METHYL)PHENYLBORONIC ACID BY FT-IR, FT-RAMAN COMBINED WITH DFT CALCULATIONS

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Literature reveals that to the best of our knowledge DFT calculations and experimental studies on molecular structure and vibrational spectra of 3-((2-isopropyl-5-methylphenoxy)methyl)phenylboronic acid (IMPMP) molecule have not been reported so far. Therefore, we have carried out detailed theoretical and experimental investigations on the molecular structure and vibrational spectra of IMPMP molecule completely. We have utilized the B3LYP [1-3] with 6-311G(d,p) basis set.

The FT-IR spectrum of IMPMP molecule is recorded in the region 4000–400 cm^{-1} on Vertex 80 spectrophotometer. The FT-Raman spectrum of IMPMP molecule has been recorded using 1064 nm line of Nd: YAG laser as excitation wavelength in the region 50-3500 cm^{-1} on the Thermo scientific DXR Raman Microscope. The calculations were performed at DFT levels by using Gaussian 09 program package, invoking gradient geometry optimization [4-5]. In order to establish the stable possible conformations, the conformational space of IMPMP molecule was scanned with theoretical methods. The optimized structural parameters were used in the vibrational frequency calculations at the DFT level to characterize all stationary points as minima. In the present work, the vibrational modes were assigned on the basis of TED analysis for 6-311G(d,p) basis set, using SQM program [6].

Keywords: Methyl -2-chloro-6-methylpridine-4-carboxlate, Molecular modeling, Density Functional Theory (DFT)

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APPLICATION OF AN OPEN-SOURCE BASED OPTICAL SENSOR PROBE FOR AN ADAPTIVE TURBIDITY AND DISSOLVED ORGANIC MATTER MONITORING

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The protection and sustainable use of marine resources require a better understanding of oceans and marine ecosystems. However, the impact of global change, the intensive use of natural resources and complex interactions between humankind and the environment show different effects on different scales. Unfortunately, current methods used in research and scientific surveys are not sufficient to address the heterogeneity and dynamics of marine ecosystems appropriately.

Therefore, a major challenge in applied environmental research is to find methods for an holistic monitoring and long-term observation technologies with increased spatio-temporal resolution. In applied research, turbidity and the content of dissolved organic matter (DOM) are key parameters to assess ecosystem health and the state of ecosystem services since they can have significant impact on light availability and materials cycle. In order to improve our understanding of such processes, more appropriate and adaptive in-situ sensor systems are needed, which are small in size and easy to deploy.

At this point, photonics and optical sensors as well as highly integrated sensor components divulge interesting opportunities to overcome the current lack of information regarding the thermophysical properties of seawater and their meaning for ecosystem services.

To this end, an open-source based optical sensor system has been developed to allow a user-specific, modular and adaptive in-situ monitoring of turbidity and the content of dissolved organic matter close to real-time. The quantification are based on attenuation or rather transmission measurements using two narrow band LEDs and corresponding detectors within the ultraviolet range (λ=370 nm, DOM content) and infrared range (λ=850 nm, turbidity) of the electromagnetic spectrum. The novelty of the sensor probe is besides the immediate digitization of all signals, the parallel water temperature and depth measurement, the possibility to have up to 200 m cable length, the self-calibration mode by using intensity modulation as well as a data provision close to real-time. Another aspect that distinguishes the proposed approach from commercially available products is the service oriented architecture of the whole system. This includes full data integration, signal processing, usability, web services and an underlying adaptive measurement principle. Besides this, the single framework architecture allows a simplified calibration of the sensor probe as well as a holistic, time and cost effective monitoring.

In cooperation with the Helmholtz-Centre for Environmental Research Leipzig (UFZ) first field experiments were conducted, latest in summer 2018, showing promising results. Currently, field campaigns are running in which the sensors are used both as stationary loggers and as mobile sensor nodes, e.g. mounted on boats. This increases the spatio-temporal resolution and improves the monitoring itself by providing the data immediately in the form of web services, e.g. by helping to faster identify „hot spots“ and "hot moments“ during field measurements.

Future goals and potential for future work are seen in particular in a closer link between in-situ monitoring and modeling of environmental processes and phenomena. This would also help to improve prediction modeling and to support decision making processes for a sustainable protection and usage of marine resources.

THE IAPWS GUIDELINE ON THE FAST CALCULATION OF STEAM AND WATER PROPERTIES WITH THE SPLINE-BASED TABLE LOOK-UP METHOD (SBTL)

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Numerical simulations of transient processes with heat-cycle calculation software, computational fluid dynamics (CFD), or thermohydraulic codes, are widely used in power engineering. During these simulations, thermodynamic and transport properties of the utilized working fluids need to be calculated extremely often. The calculation of these properties from multiparameter equations is very time-consuming and leads to inacceptable overall computing times. Therefore, property calculations are often simplified through the use of the ideal-gas equation or a cubic equation of state. Depending on the range of state, these simplifications cause inaccuracies in the results of the process simulations.

To provide more suitable property calculation algorithms for computationally intensive process simulations, the Spline-Based Table Look-up Method (SBTL) was developed in a project of the International Association for the Properties of Water and Steam (IAPWS). This method applies spline-interpolation techniques and specialized coordinate transformations to reproduce the results of an underlying formulation, e.g., the industrial formulation for water and steam IAPWS-IF97, with high accuracy and low computing time. The IAPWS Guideline contains a detailed description of the SBTL method as well as SBTL property functions of specific volume and specific internal energy (v,u), as required in CFD, and of pressure and specific enthalpy (p,h), as used in heat-cycle calculations, for water and steam. Fast and numerically consistent inverse functions of (p,v) and (u,s), as well as of (p,T), (p,s), and (h,s) are also provided. The maximum deviations of the SBTL functions from the underlying IAPWS formulations are less than 10-100 ppm. With regard to IAPWS-IF97, computations from the (v,u) spline functions are more than 130 times faster. The applicability of the SBTL method has been verified in various process simulations. The results of these simulations show negligible differences to those obtained with the direct application of IAPWS-IF97, but the overall computing times are reduced significantly.

PROPERTY LIBRARIES FOR WORKING FLUIDS FOR CALCULATING HEAT CYCLES, TURBINES, BOILERS, HEAT PUMPS, AND REFRIGERATION PROCESSES

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The program libraries for calculating the thermophysical properties for water and steam, for mixtures with water and steam, and for other working fluids are designed for practical use by engineers who calculate heat cycles, steam or gas turbines, boilers, heat pumps, or other thermal or refrigeration processes. Thermodynamic and transport properties, thermodynamic derivatives and inverse functions can be calculated.

The following property libraries are presented here:
LibIF97 for water and steam
LibIF97-META for metastable steam
LibICE for ice
LibSeaWa for seawater
LibHuGas for humid combustion-gas mixtures also at high pressures
LibHuAir for humid air also at high pressures and with high water content
LibAmWa for ammonia/water mixtures in absorption processes and the Kalina process
LibWaLi for water/lithium bromide mixtures in absorption processes
LibIdGasMix for 25 ideal gases and their mixtures
LibRealAir for real dry air
LibCO2 for carbon dioxide including dry ice
LibNH3 for ammonia
LibPropane for propane
LibButane_Iso and *LibButane_n* for iso-butane and n-butane
LibD4, *LibD5*, *LibD6*, *LibMDM*, *LibMD2M*, *LibMD3M*, *LibMD4M*, and *LibMM* for siloxanes used in ORC processes
LibCH3OH for methanol, *LibC2H5OH* for ethanol
LibH2 for hydrogen, *LibN2* for nitrogen, *LibHe* for helium and
LibSecRef for liquid coolants.

In addition, property libraries for a number of refrigerants and hydrocarbons are available.

These libraries contain the most accurate algorithms currently available for calculating thermodynamic and transport properties.

For extremely fast property computations in CFD or non-stationary process simulations, the Spline-based Table Look-up Method (SBTL) property libraries are available.

The property libraries can be used in user-specific programs written in Fortran, C++, C#, Java, Pascal (Delphi), Python, Visual Basic, or other programming languages under the operating systems Windows, Unix/Linux, or Mac OS.

Student versions of certain property libraries are available.

PROPERTY LIBRARIES FOR EXCEL, MATLAB, MATHCAD, DYMOLA, SIMULATIONX, LABVIEW, EES, SMARTPHONES, TABLETS, POCKET CALCULATORS, AND ONLINE USE

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The software developed for calculating the thermodynamic and transport properties for water and steam, mixtures with water and steam, and other working fluids have been designed for very convenient use by engineers who routinely calculate heat cycles, steam or gas turbines, boilers, heat pumps, or other thermal or refrigeration processes.

The following software solutions will be presented:
Add-In *FluidEXL*$^{\text{Graphics}}$ for Excel®
Add-On *FluidLAB* for MATLAB®
Add-On *FluidMAT* for Mathcad®
Add-On *FluidDYM* for Dymola® (Modelica) and SimulationX®
Add-On *FluidVIEW* for LabVIEW™ and
Add-On *FluidEES* for the Engineering Equation Solver® (EES).

The program *FluidDIA* was developed for calculating and plotting large-sized and camera-ready thermodynamic charts.

Steam tables are available for iPhone, iPad and iPod touch, and for Android smartphones and tablets.

The software for using steam tables and property software on Texas Instruments®, Hewlett Packard®, and Casio® pocket calculators is of particular interest for students.

Thermodynamic and transport properties of several working fluids can be online calculated using the *Fluid Property Calculator* at our website www.thermodynamics-zittau.de.

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_2.

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.

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Your research partner for combustion engines and energy systems

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Energy System Simulation

Thermophysical Properties

Fuels and Lubricants

Training, Studies and Consulting

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.

fvtr.de

FVTR Rostock GmbH • Joachim-Jungius-Str. 9 • D-18059 Rostock • **CEO: Dr.-Ing. Martin Reißig**

high precision thermoregulation

huber

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

Heating and Cooling Thermostats – Compatible Control®, MPC®, Ministat®, Variostat®

The Huber thermostat program written to model a wide range of temperatures from -90 ° C to +300 ° C.

- Hook-and bridge thermostats
- baths with polycarbonate or stainless steel baths
- Circulators for external temperature
- Refrigeration and Low Refrigerated Circulators
- Over 70 models with cooling capacities up to 7 kW

Chiller – Unichiller®, Minichiller®, RotaCool®

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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By Dieckers GmbH & Co. KG long lasting experience and the gained know-how company has become one of the leading specialist in the field of high pressure technology in a range starting from 500 bars and ending at 14.000 bars. In the field of high pressure technology as well as in the field of testing technology they offer custom made solutions to a diversity of demands. Dieckers GmbH & Co. KG scope of supply also comprises the design and manufacturing of special parts in every requested batch size.

Dieckers GmbH & Co. KG core business spans from development, design and manufacturing to the installation of high pressure components, tubing, tube-coils and complete pipe work for the industrial branches of water jet cutting, cleaning applications, hydroforming presses, chemical industry and systems for institutes of universities or research & development departments.

The high motivation, permanent availability, flexibility and reliability of company qualified team are the basis for the confidence and trust put into Dieckers by the customers in numerous industrial sectors for already over 25 years.

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.

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Turbomolecular pumps, magnetically levitated
Turbomolecular pumps, magnetically levitated
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- Ranked among top private companies
- Approximately $1.5 billion (USD) in annual sales
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- Worldwide manufacturing, distribution, and technical centers
- Sales focused by market and by region

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LEIPZIG BERLIN

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

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- 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)

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- New product development
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- 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
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- Filters
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- Hoses
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- Systematically calculates the financial value of our Swagelok’s services
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  - Emergency delivery
  - Energy management
  - Engineering services
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  - Kitting
  - Product evaluations
  - Summary billing
  - Steam audits and training
  - Swagelok weld system training
  - Vendor managed inventory

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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.

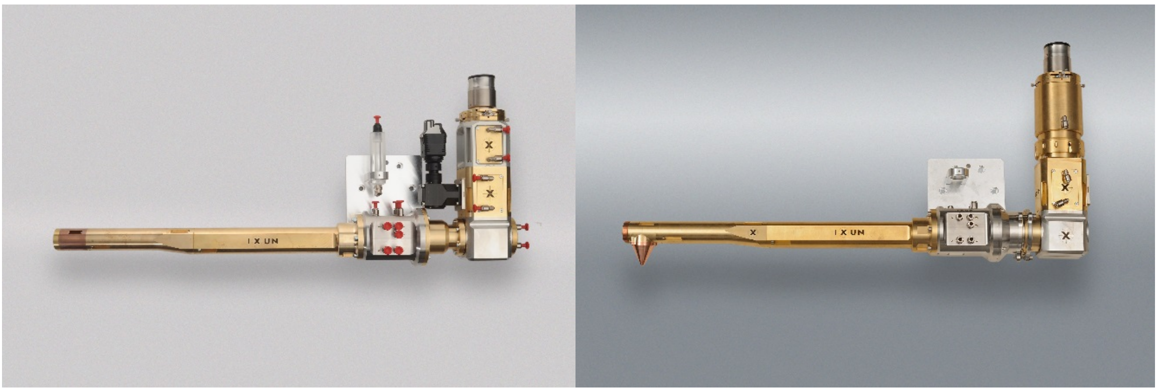
The optics have been proven for years in intensive industrial use.

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

Tool and mould construction

- Injection mould tools
- Die casting tools
- Forging tools
- Forming tools
- Fixtures

Motor construction

- Crankshafts, camshafts
- 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

TOP INDUSTRIE

High Pressure Engineering

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TOP INDUSTRIE has been a leader in the field of **High Pressure (up to 10.000 bar)** and **Temperature** for 30 years. We provide a **full range** of high pressure autoclaves, specialized equipment using pressure, high pressure valves, syringe pumps with controlled flow, testing and analysis benches, supercritical fluid systems and other devices under pressure specially designed for **Research Centers** and **Testing Laboratories.** Top Industrie is also manufacturing supercritical fluid equipment.

TOP INDUSTRIE started 30 years ago by producing high pressure components, valves, fittings and pressure generators. We have designed our own range of products and have delivered them all over the world. We then moved to the production of autoclaves and high pressure cells. A wide range of reactors from 15 ml to 10 liters, in a large variety of material and with a lot of innovative accessories; magnetic stirrer, heating and cooling, pressure control devices, injection and metering pumps…

We now design and produce full installations. Turn-key pilot units always oriented to the development of new products and new technologies. Including a wide range of new components and new processes. Gas monitoring, injection and sampling devices, Supervisory Control and Data acquisition.

TOP INDUSTRIE – YOUR HIGH PRESSURE EXPERT 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 m² test laboratory and production area, 150 m² R&D central office, with total closed area of approximately 670 m².

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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