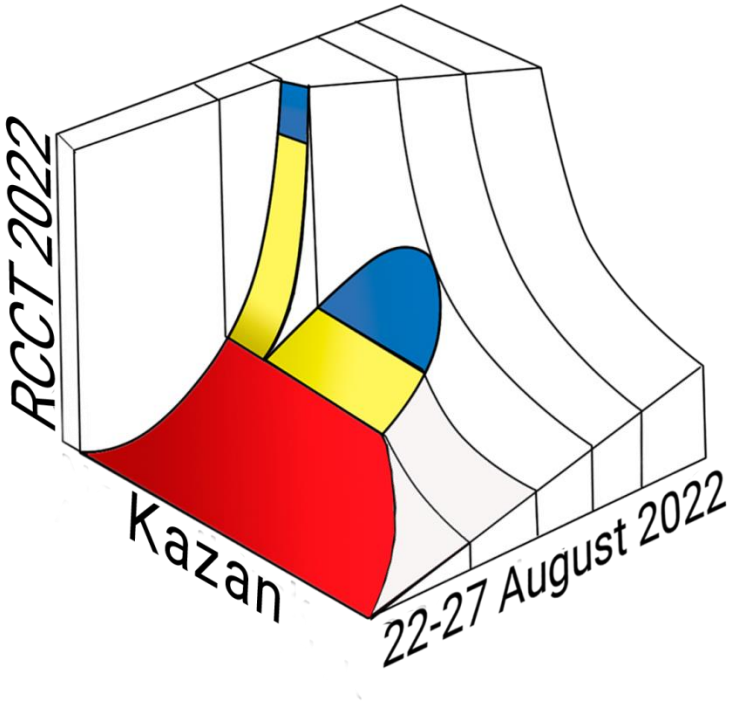
XXIII International Conference on Chemical Thermodynamics in Russia

August 22-27, 2022
Kazan, Russia



RCCT – 2022

BOOK OF ABSTRACTS

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Mendeleev Chemical Society of Russia

PREFACE

XXIII International Conference on Chemical Thermodynamics in Russia, RCCT-2022 August 22-26, 2022, Kazan, Russia: Abstracts. – Kazan, 2022. - 361 p.

This book contains the scientific program and the abstracts of presentations at the XXIII International Conference on Chemical Thermodynamics in Russia (RCCT-2022). The conferences on Chemical Thermodynamics are among the largest held in Russia since 1961. RCCT is an important scientific event not only for Russian but also for the international research community, being among the largest conferences on Chemical Thermodynamics. The conference traditionally covers all aspects of chemical thermodynamics from fundamentals to applications, including multidisciplinary approaches and related fields of science.

Until 1977 a conference of this series was called “All-Union Conference on Calorimetry" and later, until 1992, "All-Union Conference on Calorimetry and Chemical Thermodynamics". Today the RCCT International Conferences are organized every two years by large Russian scientific centers that have included Moscow (2005, 2013), Saint Petersburg (2002, 2019), Ivanovo (2007), Kazan (2009), Samara (2011), Nizhny Novgorod (2015) and Novosibirsk (2017).

This year the conference brings together more than 250 scientists from 32 cities and 15 countries; many of them are young researches, including undergraduate and graduate students. Two junior poster awards have been established by the organizers for the best poster presentations: the RCCT-2022 junior poster award “Excellence in Chemical Thermodynamics” and “Lev G. Berg award”, a special award is dedicated to the founder of theory of Differential Thermal Analysis, the first president of the International Confederation for Thermal Analysis (ICTA), professor Lev G. Berg.

The scientific program of RCCT2019 includes plenary and keynote lectures, 4 parallel sessions of oral presentations and 3 poster sessions. These contributions reflect the latest trends in Chemical Thermodynamics, including the development and application of theory, new experimental techniques and computer simulation for various systems. It is our pleasure to thank all the participants of RCCT-2022 and to welcome you in Kazan.

On behalf of the organizers,

Boris N. Solomonov, RCCT-2022 Vice-chair

THERMODYNAMIC MODELING OF LAYERED STRUCTURES BASED ON GRAPHITE OXIDE

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The subject of the study was graphite oxides (GO) synthesized by the Hammers (H-GO) and Brodie (B-GO) method. The increased interest in GO is explained by its properties: mechanical strength, hydrophility and the ability to dissolve in polar solvents. Aqueous colloidal solutions are a convenient medium for producing composites based on graphene oxide. In addition, GO posessis the ability to selectively sorb liquids. Sorption is a reproducible characteristic of the GO sample and is accompanied by swelling (an increase in interplane distances), i.e. the sorbed liquid is mainly located in the interplane space of the GO.

It is proposed to consider structures of graphite oxides B-GO and H-GO swollen in polar solvents as thermodynamic phases. The structures of the H-GO are solid solutions, the more ordered structures of the B-GO being solvates with narrow areas of homogeneity. The suggested approach made it possible for the first time to construct diagrams of the state of binary systems graphite oxide / polar solvent for systems B-GO / normal alcohol in a series from methanol to nonanol. When moving along this row, the type of the status diagram changes twice. Explained are changes in the properties of swollen structures with changes in temperature, pressure and composition. Several types of phase transitions were recorded and interpreted as incongruent melting of solvates. Transitions between different heterogeneous regions of the state diagram were experimentally observed.

The behavior of the systems observed in our experiments was described using diagrams of three types. In the diagram of the first type there are two solvates (I and II). This diagram describes the systems B-GO / methanol and ethanol. Systems B-GO / butanol, pentanol, hexanol, heptanol are described by a diagram of the second type. Solvates I, II and III are present here. Finally, five solvates I-V are shown in diagrams of the state of B-GO / octanol and nonanol. The designation of solvates in different systems with the same Roman numeral indicates the same internal structure of the solvate. A layered model of the structure of swollen B-GO structures was proposed (parallel layers of polar liquid between the planes of graphite oxide). For example, structure III contains three "layers" of polar liquid between adjacent planes of graphite oxide. The "layer" is characterized by the amount of sorption. The appearance of a new "layer" of liquid increases the interplane distance by a certain amount.

It is shown that solvates I, III, V are stable, and solvates with an even number of layers are less stable. II melts incongruently when heated and solvate IV is detected only in a narrow temperature range in 1-octanol and 1-nonanol systems.

Phase diagrams summarize our experimental data obtained by DSC method, isopiestic and isothermal TG (boundaries of phase regions). The phases were identified by XRD method in equilibrium and nonequilibrium experiments.

For the first time, the existence of two types of similar phase transitions, differing in temperature and enthalpy of transformation, was noted. In the first case, a liquid layer in contact with the graphene plane is incongruently melted (a typical example is CH_3OH), in the other, a layer located in the center of the sorbed liquid mass ($C_8H_{17}OH$ and $C_9H_{19}OH$). In the second case, the transition temperature is close to the melting temperature of the sorbed liquid (+5-10 degrees), in the first case, the difference can be up to +110 degrees.

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