



Condensed Matter and Interphases (Kondensirovannye sredy i mezhfaznye granitsy)

Аннотации на английском языке

Review

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Random First Order Transition from a Supercooled Liquid to an Ideal Glass (Review)

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Abstract

The random first order transition theory (RFOT) describing the transition from a supercooled liquid to an ideal glass has been actively developed over the last twenty years. This theory is formulated in a way that allows a description of the transition from the initial equilibrium state to the final metastable state without considering any kinetic processes. The RFOT and its applications for real molecular systems (multicomponent liquids with various intermolecular potentials, gel systems, etc.) are widely represented in English-language sources. However, these studies are practically not described in any Russian sources. This paper presents an overview of the studies carried out in this field.

Keywords: supercooled liquid, ideal glass, distribution functions, replicas, random first order transition.

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Computer Simulation of Sorption Interactions of L-Arginine and L-Lysine with Carbon Nanotubes

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Abstract

Carbon nanotubes (CNTs) are a new class of nanomaterials with a high potential for different technological applications. The prospects of using them in biomedicine is associated with the ability of CNTs to cross the cell's membrane without

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being impaired, which determines the significance of the study of the interactions of CNTs with biologically active substances, especially amino acids. This work presents a computer simulation of the structure and characteristics of arginine (lysine) – single-wall carbon nanotube (CNT) systems using the B3LYP/6-31G(d,p) density functional theory with GD3 dispersion correction. We calculated the energies of adsorption, dipole moments, total charge on the amino acid and nanotube atoms, and the smallest distances from the amino acid atoms to the CNT. Taking into account the dispersion correction, which is almost absent in scientific literature, allows more accurate calculations of the energies of adsorption of amino acids on CNT to be obtained as compared to the existing calculations due to the high polarizability of CNTs. We considered scenarios with the amino acid position on the open end and on the external and internal lateral surfaces of the CNT. The calculated series of adsorption energies satisfies the conditions $E_{\text{end}} > E_{\text{inside}} > E_{\text{lateral}}$. This is due to the fact that when the amino acid is placed on the external lateral surface of a CNT the sorbate interacts with a part of the lateral surface of the tube. When it is placed inside the CNT the sorbate interacts with the whole surface through van der Waals forces and when the sorbate is placed on the end of the sorbent a covalent bond is formed between them. The formation of the covalent bond on the open end of the CNT is due to the higher electron density near the ends of the nanotube as compared to the external and internal lateral surfaces of the tube. An explanation is given of the mechanisms of adsorption and enhancement of the antibacterial action of the CNT functionalised by arginine and lysine, as compared to nonfunctionalised CNTs.

Keywords: carbon nanotubes, amino acids, computer simulation, adsorption.

Funding: The study was conducted within the framework of the government order for higher education institutions in the sphere of scientific research for years 2020–2022, project No. FZGU-2020-0044.

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Thermodynamic investigation of the Bi_2Se_3 – Bi_2Te_3 system by the EMF method

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Abstract

Binary and complex chalcogenides with a tetradimite-like layered structure are of great practical interest as topological insulators, thermoelectric, and optoelectronic materials. Their fundamental thermodynamic functions in combination with phase diagrams are important for the development and optimization of methods for the synthesis and growth of crystals. The work presents the results of a thermodynamic study of the starting compounds and solid solutions of the Bi_2Se_3 – Bi_2Te_3 system using the method of electromotive forces (EMF). Various modifications of this method are widely used to study binary and complex metal chalcogenides. Studies were carried out by EMF measurements of the concentration chains of the following type:

(–) Bi (solid) | ionic liquid + Bi^{3+} | Bi in the alloy (solid) (+)

in the temperature range 300–450 K.

The pre-synthesized equilibrium $\text{Bi}_2\text{Se}_{3-x}\text{Te}_x$ alloys ($x = 0; 0.6; 1.2; 1.8; 2.0; 2.4; 3.0$) with a 0.5 at% excess tellurium were used as right electrodes. Ionic liquid (morpholine formate) with the addition of BiCl_3 was used as the electrolyte.

The acquired experimental data were processed by the Microsoft Office Excel 2003 computer program using the least-squares method and linear equations of the type $E = a + bT$ were obtained. The obtained equations of the EMF temperature dependences were used to calculate the relative partial molar functions of bismuth in the alloys. The diagram of solid-phase equilibria of the Bi–Se–Te system was used to determine the equations of potential-forming reactions and the latter were used to calculate the standard thermodynamic functions of the formation and standard entropies of Bi_2Se_3 , Bi_2Te_3 compounds and $\text{Bi}_2\text{Se}_{3-x}\text{Te}_x$ solid solutions of the above compositions. The thermodynamic functions of the formation of $\text{Bi}_2\text{Se}_{3-x}\text{Te}_x$ solid solutions from the initial binary compounds were also calculated. The results correlate well with the structural data that suggests some ordering in the arrangement of selenium and tellurium atoms in the b-phase crystal lattice of the

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Bi_2SeTe_2 composition: selenium atoms predominantly occupy the central layer of the five-layer, and tellurium atoms are located in the two outer layers.

Keywords: bismuth selenides, bismuth telluride, solid solutions, EMF method, thermodynamic properties.

Funding: The work has been carried out within the framework of the international joint research laboratory “Advanced Materials for Spintronics and Quantum Computing” (AMSQC) established between Institute of Catalysis and Inorganic Chemistry of ANAS (Azerbaijan) and Donostia International Physics Center (Basque Country, Spain) and partially supported by the Science Development Foundation under the President of the Republic of Azerbaijan, a grant EİF/MQM/Elm-Tehsil-1-2016-1(26)-71/01/4-M-33.

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Cathodic Deposition of Zinc-Nickel Coatings from a Dilute Ammonium Chloride Electrolyte with a High Glycine Concentration

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Abstract

This study determined the kinetics of the synthesis, the chemical composition, and morphology of zinc-nickel coatings electrolytically obtained from low-concentration (0.04 M ZnCl_2 , 0.08 M NiCl_2) ammoniacate and ammonia-glycinate chloride solutions. Transient electrochemical methods (cyclic voltammetry and linear sweep voltammetry) allowed us to determine that the cathodic deposition of Zn–Ni alloy coatings, regardless of the presence of glycine in the ammonium chloride electrolyte, is limited by the stage of diffusion mass-transfer of ions, whose electrochemical reduction (the charge transfer stage) is irreversible. The introduction of relatively high concentrations of glycine (0.3 M) in the electrolyte allows obtaining smoother coatings, which is demonstrated by the results of scanning electron microscopy. At the same time, energy dispersive X-ray spectroscopy demonstrated that the atomic fraction of nickel in the potentiostatically deposited coating increases on average by 9.7%. It is possible that the alteration of the chemical composition results in a significant decrease (on average by ~15 %) in the current efficiency in electrolytes with glycine, since it catalyses the side reaction of hydrogen evolution.

Keywords: electrodeposition, zinc-nickel coatings, ammine electrolyte, glycine, current efficiency, voltammetry.

For citation: Kozaderov O. A., Tinaeva K. E., Tinaeva A. E., Burliaev D. V. Cathodic deposition of zinc-nickel coatings from a dilute ammonium chloride electrolyte with a high glycine concentration. *Kondensirovannye sredy i mezhfaznye granitsy = Condensed Matter and Interphases*. 2020; 22(3): 320–326. DOI: <https://doi.org/10.17308/kcmf.2020.22/2962>

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Usage of the Kolmogorov–Johnson–Mehl–Avrami Model for the Study of the Kinetics of the Formation of Natural Gas Hydrate in Inverse Oil Emulsions.

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Abstract

The article presents the results of a study of the hydration of the aqueous phase in inverse oil emulsions with natural gas rich in methane (more than 90 vol.%). The aim of the work was to study the kinetics of the crystallisation of oil emulsions during the formation of natural gas hydrates in them using the method of differential scanning calorimetry (DSC).

The objects of the study were inverse oil emulsions containing 20, 40, 60, and 80 wt% of water. DSC is used under quasi-equilibrium experiment conditions to study the kinetics of hydration of oil emulsions with gas.

The study showed the applicability of the Kolmogorov–Johnson–Mehl–Avrami model (KJMA) in order to describe the crystallisation process of inverse oil emulsions in a quasi-equilibrium DSC experiment. The kinetic parameters of the KJMA model in emulsions were determined for the processes of water drops conversion into ice, as well as their hydration with natural gas. It was shown that within the system “natural gas-oil-water” the process of ice formation is characterised by high values of the Avrami exponent ($n > 3$) and the degree of freedom ($\lambda = 3$), and the process of natural gas hydrate formation is characterised by low values of the Avrami exponent ($n < 3$) and medium degree of freedom ($\lambda = 1-3$). It was shown that in a continuous aqueous phase, natural gas hydrates are formed by instantaneous nucleation in the form of separate one-dimensional crystals; while in oil, hydrates are nucleated at a constant rate and, depending on the water content, grow in the form of disparate crystallites, shell, or spherulites. The obtained research results make it possible to deepen our knowledge of the kinetics and hydration mechanisms in oil emulsions, they can be used to complement the scientific basis for creating new technologies for the joint transportation of oil and hydrated natural gas in it.

Keywords: crystallisation, kinetics, Kolmogorov–Johnson–Mehl–Avrami model, differential scanning calorimetry, oil emulsion, natural gas hydrate, hydrate formation.

Funding: The study was supported by state-funded research, development, and engineering project No. AAAA-A17-117040710035-7.

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Synthesis and characterisation of ternary molybdates $\text{AgZn}_3\text{R}(\text{MoO}_4)_5$ ($R = \text{In, Fe}$)

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Abstract

An important role in the study and the obtaining of new phases with valuable physical and chemical properties is taken by ternary compounds with a tetrahedral anion containing various combinations of mono- and multivalent cations, including ternary molybdates and tungstates. Silver ternary molybdates $\text{AgA}_3\text{R}(\text{MoO}_4)_5$ with the $\text{NaMg}_3\text{In}(\text{MoO}_4)_5$ structural type (triclinic crystal system, space group $\text{P}\bar{1}$, $Z = 2$) are of particular interest and have a high ion conductivity (10^{-3} – 10^{-2} S/cm). In this regard, the aim of this work was to reveal the possibility to form similar compounds in silver, zinc, indium, and iron molybdate and tungstate systems and to determine the effect of the nature of tetrahedral anion and three-charged cations on their obtaining and properties.

Polycrystalline samples were synthesized using a ceramic technology and studied by differential thermal (DTA) and X-ray diffraction analysis (XRD).

The research resulted in obtaining a new ternary molybdates $\text{AgZn}_3\text{R}(\text{MoO}_4)_5$ ($R = \text{In, Fe}$) crystallising in the triclinic crystal system (space group $\text{P}\bar{1}$, $Z = 2$). The sequence of chemical transformations that occur during the formation of these compounds, their crystallographic and thermal characteristics were determined. Unit cell parameters for the indium compound are as follows: $a = 6.9920(4)$, $b = 7.0491(4)$, $c = 17.9196(9)$ Å, $\alpha = 87.692(5)$, $\beta = 87.381(5)$, $\gamma = 79.173(5)^\circ$; and for the iron compound: $a = 6.9229(3)$, $b = 6.9828(4)$, $c = 17.7574(8)$ Å, $\alpha = 87.943(4)$, $\beta = 87.346(5)$, $\gamma = 78.882(5)^\circ$. It was established that silver-containing ternary zinc tungstates with indium and iron with a similar structure are not formed.

Keywords: ternary molybdates, silver, tungsten, solid-state synthesis, X-ray diffraction analysis (XRD), thermal properties.

Funding: The study received financing within the framework of state order No. 0339-2019-0007 to the Baikal Institute of Nature Management, Siberian Branch of the Russian Academy of Sciences. It was partially funded by the Russian Foundation for Basic Research (project No. 16-03-00510 a).

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Kinetics of Phase Transformations during Selective Dissolution of Cu_5Zn_8

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Abstract

The study determined the kinetics of the selective anodic dissolution of the copper-zinc intermetallic compound Cu_5Zn_8 (gamma-phase) in an acetate buffer solution. Microscopic and X-ray analysis methods demonstrated the selective nature

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of the corrosive dissolution of Cu_5Zn_8 . The dissolution results in the dezincification of the intermetallic compound and morphological development of its surface accompanied by the formation of the copper phase. A theoretical model of the transition of the electrode surface to the critical state together with the experimental concentration dependencies of the critical potential and critical overvoltage demonstrated that the dissolution of zinc from Cu_5Zn_8 is most probably limited by the non-stationary diffusion mass-transfer in the solid phase of the intermetallic compound. The study also demonstrated that the phase transformation during the overcritical selective anodic dissolution of the gamma-phase of Cu_5Zn_8 in an acetate environment accelerates following the growth of the anodic potential and is controlled by the surface diffusion of adatoms towards the three-dimensional nucleus of the copper phase with instantaneous nucleation.

Keywords: copper-zinc alloy, gamma phase, selective dissolution, phase transformation, surface development, heterogeneous nucleation.

For citation: Kozaderov O. A., Taranov D. M., Krivoshlykov A. N., Borodkina S. V. Kinetics of phase transformations during selective dissolution of Cu_5Zn_8 . *Kondensirovannye sredy i mezhfaznye granitsy = Condensed Matter and Interphases*. 2020; 22(3): 344–352. DOI: <https://doi.org/10.17308/kcmf.2020.22/2965>

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Obtaining Iron (III) – Containing Triple Molybdate $\text{K}_5\text{FeZr}(\text{MoO}_4)_6$ by Sol-Gel Technology

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Abstract

Oxide compounds, as the basis of promising materials, are used in various fields of modern technologies due to their electrical and optical properties. Some of them, possessing a combination of ferroelectric, scintillation, electrical, and optical properties, are being studied as promising materials for electronics. In this case, their dispersion plays an important role.

Traditionally, the synthesis of oxide compounds is carried out by ceramic technology. More promising for the synthesis of fine powders are the methods of “soft” chemistry, among which we have identified and applied the sol-gel method. In this method, “mixing” occurs at the molecular level, which contributes to an increase in the reaction rates and a decrease in the synthesis temperature. The method involves the use of inorganic salts as precursors in combination with complexing agents (citric acid). The use of such precursors allows one to achieve high uniformity at relatively low temperatures. A feature of this approach is the use of fewer organic compounds: an aqueous solution of citric acid is used as a chelating agent. The aim of this work was to obtain triple molybdate by sol-gel technology (SGT) based on the example of iron-containing potassium zirconium molybdate.

The iron-containing triple potassium zirconium molybdate was obtained using the of citrate sol-gel technology and solid-phase synthesis (SPS) methods. The triple molybdate obtained by two methods was characterized by X-ray phase analysis, DSC, and impedance spectroscopy.

The developed sol-gel synthesis technique allowed lowering the synthesis temperature, to obtain triple molybdate with high values of homogeneity, dispersion, and electrical conductivity. This technique can be used to obtain double and triple zirconium (hafnium) molybdates containing a trivalent cation.

Keywords: iron-containing, triple molybdate, zirconium, potassium series, sol-gel synthesis.

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Quantum Chemical Modelling of the Scandium Sub-Group Metal Endofullerenes

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Abstract

Endofullerenes with one or several metal atoms inside the carbon cage (metallofullerenes) are of considerable practical interest as promising basic materials for creating highly effective contrasting agents for magnetic resonance imaging (MRI) as well as antioxidant and anticancer drugs. These compounds can also be used in spintronics to build nanoscale electronic devices. In the framework of the density functional theory, this work presents a calculation of the structural, electronic, and thermodynamic characteristics of scandium sub-group metal endofullerenes with the number of encapsulated atoms from one to seven in the gaseous phase. The stable structures with symmetries C_3 , C_2 , C_3 , and C_1 , were described. They correspond to the positions of the metal atoms inside the fullerene cage. The theoretical limit for the number of metal atoms at which the endofullerene structure remains stable is six atoms for scandium, four for yttrium, and three for lanthanum. The calculations showed that the most stable structures are the ones with two and three encapsulated atoms. The relationship between the number of encapsulated atoms and the nature of electron density distribution were described. The total charge on the encapsulated metal cluster is positive for $Me@C_{60} - Me_3@C_{60}$ compounds, weakly positive for $Me_4@C_{60}$ (some of the atoms have negative charge), and negative for $Me_5C_{60} - Me_6@C_{60}$ compounds. The spin leakage effect was described for the structures with a doublet spin state. As for the endofullerenes with three and more encapsulated atoms, this effect is insignificant, which makes the creation of contrasting agents for MRI based on them impractical.

Keywords: endofullerenes, metallofullerenes, quantum chemical calculations, density functional theory, molecular symmetry, spin leakage.

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Hydration and Intermolecular Interactions in Carboxylic Acids

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Abstract

At the moment, the most accurate and reliable information about intermolecular interactions in low-molecular compounds and their polymer analogues can be obtained by means of combined UV, visible, and IR spectroscopy. However, this combination is not always used when interpreting the results of intermolecular interactions in carboxylic acids. Therefore, the aim of our study was to investigate the intermolecular interactions in carboxylic acids and their hydration properties using the UV, visible, and IR spectroscopy.

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The article presents the results of the investigation of intermolecular interactions and hydration in carboxylic acids by means of UV, visible, and IR spectroscopy, and the microscopic study of the swelling/contraction curves of the beads of the sorbents with slightly acidic –COOH groups in exchange reactions of $R-COOH + NaOH \leftrightarrow R-COO^-Na^+ + H_2O$. The study revealed a H-bond in the water dimers formed due to the Coulomb, exchange, charge transfer, polarisation, and dispersion components of the total energy of the hydrogen bonds. In our study we also tested the formulas for the calculation of the energy of the H-bond, enthalpy, the force constants of the H-bond, and the elongation of the covalent bond. The article suggests a formula for calculating the distance $R_{CH_2...O}$, i.e. the length of the H-bond between the donor and the acceptor of the proton, based on the information about stretching vibrations in the IR spectra of carboxylic acids. We also specified the characteristic frequencies of the stretching and deformation vibrations of certain H-bonds and functional groups in fatty acids. The article demonstrates the possibility of the formation of five- and six-membered cycles, resulting from the formation of H-bonds between CH_2 groups of the chain and –COOH end groups of carboxylic acids.

The characteristic electron and vibrational frequencies in the UV and IR spectra were used to determine the intermolecular interactions in ion exchangers CB-2 and CB-4. The microscopic and microphotographic study of the swelling of certain beads of carboxylic cationites helped to register the presence of the outer shell $R-COO^-...Me^+$ and the inner shell $R-COOH$ during the exchange reactions: $R-COOH + Me^+ + OH^- \leftrightarrow R-COO^-...Me^+ + H_2O$.

Keywords: UV spectroscopy, IR spectroscopy, visible spectroscopy, carboxylic acids, intermolecular interactions.

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Solid Dosage Forms of Nootropic Action Based on Pantogam and Succinic Acid

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Abstract

In recent years, research related to the search and study of the mode of action of new and used in medicine nootropic agents has been carried out at a high rate. The research related to the search for new combined drugs of nootropic action based on the substances of d-gamma-Pantothenate of calcium and succinic acid, which have neurometabolic, atigipoxic, and adaptogenic properties, is of interest. The purpose of this study was to develop and justify the optimal composition and manufacturing technologies of tablets with nootropic effect and standardise the proposed dosage forms containing Pantogam and succinic acid.

The method for preparing the tablet mixture is as follows: all components were weighed in the required amount, Pantogam was placed in the mortar, then succinic acid was added and ground to a consistent white powder. The tablets were pressed on a manual press at a pressure of 120 mn/m². The coating was applied on a laboratory fluidised bed unit with a single nozzle in a perforated drum with a volume of 1000 ml. The obtained tablets were evaluated according to the requirements for State Pharmacopoeia XIII and State Pharmacopoeia XIV. The comparison of the Pantogam tablets with succinic acid obtained by direct pressing and by wet granulation showed that the method of direct pressing allows obtaining tablets with good physical and mechanical properties and bioavailability. The methods based on acid–base titration and spectrophotometric determination were developed for the quantitative determination of Pantogam in tablets. The method of quantitative determination of succinic acid in dosage forms was validated.

Based on the study of physicochemical and technological properties of substances and excipients, the compositions and technology for obtaining tablets containing Pantogam and succinic acid were justified and developed. It was found that

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solid-phase interactions occur with the combined presence of Pantogam and succinic acid in the tablets. The methods of qualitative and quantitative analysis of dosage forms containing Pantogam and succinic acid based on complexometric titration and high-performance liquid chromatography were developed. The procedure of validation of the method for determining succinic acid by HPLC in the developed dosage forms confirmed the validity of the proposed method.

Keywords: Pantogam, succinic acid, tablets, complexometry, high-performance liquid chromatography, validation.

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Possibilities and peculiarities of spray technologies in organic synthesis

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Abstract

Size effects considerably change the state and physicochemical properties of dispersal systems. The peculiarities of chemical processes occurring in small (nano, pico, and femtolitre) volumes are of a great importance for the production technologies of unique materials. The aim of this work was the experimental confirmation of size effects during chemical processes in small volumes and their interpretation based on the concepts of chemical thermodynamics.

The object of the study consisted in reactions of organic synthesis conducted in ensembles of sessile drops formed by aqueous solutions of organic compounds with the participation of a gaseous medium. The methods of optical microscopy with digital image processing were used for observation. The experiments definitely demonstrate the influence of geometric parameters (radius, contact angle) on the kinetics of phase and chemical transformations in polydisperse ensembles of sessile drops of organic and aqueous-organic mixtures interacting with volatile reagents in a gaseous medium. These features are manifested in the kinetics of changes in the size of drops as well as in the morphology of products obtained by their evaporation.

The interpretation of size effects in the framework of equilibrium chemical thermodynamics explains the shifts in chemical equilibrium and changes in the reaction rate. The equilibrium conditions arising in drops of different volumes during mass transfer with the gas phase were described. It is stated that the most important factor in the processes of organic synthesis using spray technologies is the high surface activity of organic substances. Comprehension and practical application of these peculiarities allows adjusting the reaction rate, improving the mutual solubility of partially miscible reagents, and affecting the composition and properties of the final product.

Keywords: organic synthesis in spray, size effects, chemical equilibrium constants, liquid-vapour equilibrium, nanoreactor.

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