

V. Karazin Kharkiv National University

International Conference

***Modern Physical Chemistry
for Advanced Materials***

devoted to the 100th anniversary of the birth of Professor Nikolai Izmailov

June 26-30 2007

B O O K o f A B S T R A C T S

Kharkiv

International conference MODERN PHYSICAL CHEMISTRY FOR
ADVANCED MATERIALS (MPC'07), devoted to the 100th
anniversary of the birth of Professor Nikolai Izmailov / Book of
abstracts: Kharkiv, Ukraine. 26-30 June, 2007, 399 p.
ISBN 966-623-442-4

*Original author's style including interpretation of formulas and
names of chemical compounds, schemes, pictures and explanations,
is preserved in the abstract published in this book.*

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**MODERN PHYSICAL CHEMISTRY FOR ADVANCED
MATERIALS
MPC'07**

organized by

V. Karazin Kharkiv National University

in cooperation with

L. M. Litvinenko Institute of Physico-Organic Chemistry and
Coal Chemistry of National Academy of Sciences of Ukraine

and

Physical Chemistry Department of Ukrainian Chemical Society

under the auspices of

IUPAC (International Union of Pure and Applied Chemistry)

National Academy of Sciences of Ukraine

European Association for Chemical and Molecular
Sciences (EuCheMS)

Sponsored and supported by:

- Alumni Association of V. Karazin Kharkiv National University
- State Scientific Institution "Institute of Single Crystals"
- Scientific Council of Analytical Chemistry of National Academy of Sciences of Ukraine
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- An anonymous sponsor from Russia

COMBINED MICROCALORIMETRIC AND SORPTION-ANALYTIC STUDIES OF ION EXCHANGE THERMODYNAMICS ON MORDENITE

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Combined sorption-analytic studies of ion exchange equilibria and direct microcalorimetric measurements of ion exchange heats of K^+ and Ca^{2+} cations were performed on Na-forms of two natural mordenites (M): mainly calcium mordenite from Vodica deposit (Transcarpathia) and mostly sodium mordenite from Karadag deposit (Crimea). The ion exchange was studied in static conditions (S:L = 100) in aqueous solutions of Na^+ , K^+ and Ca^{2+} chlorides at constant ionic force $I = 0.1$ and various proportions (10 variants) of exchange cations. The integral heats of ion exchange were measured in similar conditions using the Calve microcalorimeter (Setaram, France) equipped with specially designed measuring cell.

The ion exchange isotherms exhibit high selectivity of the two mordenite samples with respect to K^+ cations. For the exchange systems involving Ca^{2+} ions, the ion exchange isotherms exhibit the change of selectivity at certain degree of exchange.

At low concentrations of Ca^{2+} ions in the solution, the two samples exhibit pronounced selectivity with respect to these ions; at higher concentrations the zeolites become more selective to Na^+ cations. It is to be noted that the amount of Ca^{2+} ions sorbed by Vodica mordenite (which possesses large number of extraframework cations) is by a factor of two higher than that adsorbed by Karadag mordenite. This fact can be explained from structural considerations: by the memory effect of mordenite with respect to the extraframework cations which were present during the natural crystallisation of the mineral.

The exchange of K^+ ions on both samples is accompanied by the release of heat in the entire occupation range. For the Ca^{2+} -NaM system of Vodica deposit the exothermal exchange was observed only at $\theta \leq 0.2$. The Karadag mordenite is characterised mainly by negative exchange heats ($\Delta H > 0$).

From the experimental data, the variations of integral molal free energies ΔG_m and entropies ΔS were calculated in the entire range of solid phase occupation θ by sorbed cation. It was shown that the free energy of exchange in the K^+ -NaM system is determined by the enthalpy constituent, and in the Ca^{2+} -NaM system – by the entropy constituent.

MOLECULAR AND ELECTROLYTE SOLUTION SYSTEMS IN FIRE SUPPRESSION

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Among solvents existing on the Earth water is the cheapest and accessible fire extinguishing substance, but it has insufficient extinguishing ability, which is lower than calculated. For increase of extinguishing properties of water it is offered to add substance of the different nature in water. There is too much information on the given problem in scientific literature, but in many cases it is rather difficult for the analysis. Therefore in work it is made on attempt of generalization of this information for establishment of interrelation between physical and chemical properties of solutions and time of extinguishing (τ).

Typical for fires in residence sector is a burning of wood and cellulose products (class A fires). According to the analysis of existing papers about extinguishing efficiency of water it is more often offered to use solutions of electrolytes and high-molecular compositions. The action of different by the nature additives is different. Addition of polymeric impurities essentially influence on the period of extinguishing of the fire at small concentration [1]. At concentration more than 2-3 %_{weight} the time of extinguishing increases, therefore the mixture with concentration more than 5%_{weight} is not expedient for extinguishing. Addition of electrolytes is effective only at the high concentration (10-20 %_{weight}). The last is caused by the fact that electrolytes in two-componental mixture influence on a superficial tension (σ) and viscosity (η) insignificantly,

and at the high concentration the dominating role is got with effect of inhibition of cathalatik centers of a flame.

Optimum concentration of surface-active substances (SAS) in solutions makes 0,25-0,5 %_{weight}. The superficial tension essentially decreases only at concentration of impurity up to 1 %_{weight}. In two-componental mixture (the second component - SAS) σ does not decrease below for $(27-30)10^{-3}$ N/m. It is caused by gradual growth of amount of SAS molecules on surface split of phases. Time of extinguishing essentially depends on viscosity of a solution so at increase η on $(2-3)10^6$ m²/s time of extinguishing decreases in 3-4 times. Optimum for extinguishing of wood by two-componental mixture is η $(4-5)10^6$ m²/s [2]. The indicated optimum viscosity is

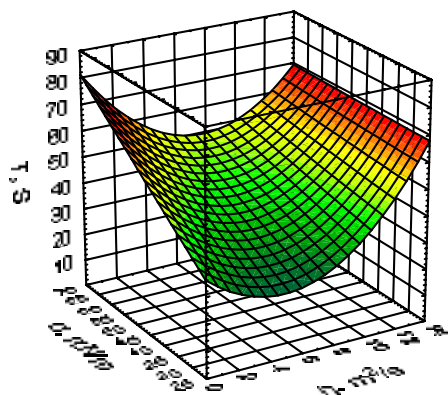


Fig. 1 Dependence of extinguishing time on physical and chemical properties of extinguishing compositions (σ , η).

Using the additive of one nature, corrects only one parameter of extinguishing composition. Only use of the combined additives (polymeric substance + low-molecular SAS + electrolyte) gives optimum values the basic physical and chemical properties of a composition (fig. 1). From figures it is obviously, that during extinguishing in which effect of inhibition is absent, to achieve time of extinguishing class A fire less than ~ 20 s is impossible at any concentration of additives.

However it is necessary to take into account, that the given dependence is submitted for temperature 20°C. At ingress extinguishing substances in a zone of burning viscosity of solutions is

reduced in 2-3 times whereas the superficial tension decreases insignificantly - on $(10-15)10^{-3}$ N/m.

For decrease of extinguishing time it is effective to use homogeneous solutions - emulsion. Halogenhydrocarbons with temperature of boiling <373 K, which at ingress in a zone of burning boil and increase dispersiveness of a stream of extinguishing solution are as a disperse phase. At extinguishing by means of emulsion efficiency increases by means of inhibition by halogenhydrocarbons and the large heat-conducting surface.

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FAVORABLE BINDING SITES AND LOCALIZATION OF PYRROLOQUINOLINE ANALOGUES IN A DPPC BILAYER FROM MOLECULAR DYNAMICS SIMULATIONS

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A series of heteroazaaromatic compounds, composed of pyrrolo- and quinoline moieties has revealed an interesting phenomenon of solvent-catalyzed excited-state tautomerization [1]. The electronic excitation of such a system induces significant intramolecular transfer of electron density from an H-bond donor (pyrrole) to an acceptor (quinoline) parts of a chromophoric system. The remarkable and cooperative acid-base changes, which occur on opposite parts of the excited chromophore, introduce also a driving force for the proton transfer reaction. In the presence of some appropriate protic solvents, H-bond donor-acceptor bifunctional

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Наукове видання

Сучасна фізична хімія
для хай-тек матеріалів
(збірка тез доповідей)

Комп'ютерна верстка Пантелеймонов А. В.
Макет обкладинки Дончик І. М.

61077, Харків, пл. Свободи, 4,
Харківський національний університет
імені В. Н. Каразіна,
організаційно-видавничий відділ НМЦ

Підписано до друку 16.06.2007. Формат 60x84/16.
Папір офсетний. Друк ризографічний
Обл.-вид. арк. 30,0. Умов.-друк. арк. 32,5.
Наклад 200 прим. Ціна договірна.

Надруковано ФОП «Петрова І. В.»
61144, Харків-144, вул. Гв. Широнінців 79^Б, к. 137
Тел. 362-01-52

Свідоцтво про державну реєстрацію ВОО № 948011
від 03.01.2003