



## Vol. 11, No. 2, 2017

A simultaneous English language translation of this journal is available from Pleiades Publishing, Ltd.  
Distributed worldwide by Springer. *Russian Journal of Physical Chemistry B* ISSN 1990-7931.

### Elementary Physicochemical Processes

Mathematical Modeling of the Dynamics of Photoreactions  
of a Five-Level Molecule

*V. A. Morozov, Yu. M. Dubina, and E. A. Smolenskii* 199

### Structure of Chemical Compounds. Spectroscopy

Diagonal *N*-Representability as a Method for Solving the Representability Problem

*M. M. Mestechkin* 208

Selective Excitation of Single Lines of a Multiplet for Interpretation of Spectra  
of Complex Multicomponent Systems

*G. S. Borodkin, I. G. Borodkina, Yu. E. Chernysh,  
M. G. Morozov, V. T. Panyushkin, and V. A. Volynkin* 228

EPR Spectroscopic and X-Ray Diffraction Studies of Carbon Fibers  
with Different Mechanical Properties

*A. L. Kovarskii, V. V. Kasparov, A. V. Krivandin, O. V. Shatalova,  
R. A. Korokhin, and A. M. Kuperman* 233

### Influence of External Factors on Physicochemical Transformations

Effectiveness of Charge Separation from the Long-Lived Second  
Excited State of Donors

*S. V. Bazlov, S. V. Feskov, and A. I. Ivanov* 242

### Kinetics and Mechanism of Chemical Reactions. Catalysis

Comparison of the Process of Deactivation of Homogeneous Catalysts by the Example  
of Copper(II) Compounds in the Presence of Some Additives in Various Solvents

*L. A. Smurova* 249

Catalytic Oxidation of Hydrogen on the Surface of Quartz, Stainless Steel,  
and MgO Near the Third Ignition Limit

*S. N. Kozlov, E. A. Markevich, and E. N. Aleksandrov* 255

### Combustion, Explosion, and Shock Waves

Calculation of Shock Wave Propagation in Water Containing Reactive Gas Bubbles

*K. A. Avdeev, V. S. Aksenov, A. A. Borisov, D. G. Sevastopoleva, R. R. Tukhvatullina,  
S. M. Frolov, F. S. Frolov, I. O. Shamshin, B. Basara, W. Edelbauer, and K. Pachler* 261

Formation of Titanium and Niobium Aluminides Induced by Hydrogen in a Hydride Cycle

*S. K. Dolukhanyan, O. P. Ter-Galstyan, A. G. Aleksanyan,  
G. N. Muradyan, and N. L. Mnatsakanyan* 272

Micro-Hot-Spot Model Taking into Account the Temperature Dependence  
of the Laser Pulse Absorption Efficiency Factor

*A. V. Kalenskii, A. A. Zvekov, and A. P. Nikitin* 282

Laws Governing the Combustion of the Ni + Al System under a Low Ambient Gas Pressure

*N. A. Kochetov and B. S. Seplyarskii* 288

## Electric and Magnetic Properties of Materials

An Aerodynamic Model of the Collisional Alignment of the Cations of Macromolecules

*M. N. Levin, I. Yu. Kretinin, V. E. Chernov, and B. A. Zon*

294

---

## Chemical Physics of Biological Processes

Dependence of the Rate of Growth of *Aspergillus niger* Microscopic Fungi on the Kinetic Parameters of the Adhesion of Their Spores to Polymeric Materials

*I. G. Kalinina, K. Z. Gumargalieva, V. V. Kazarin, and S. A. Semenov*

304

Ab Initio and QSAR Study of Several Etoposides as Anticancer Drugs: Solvent Effect

*R. Sayyadi kord Abadi, A. Alizadehdakhel, and S. Dorani Shiraz*

307

Equilibrium and Kinetics of Biosorption of Oxalic Acid by Wheat Straw

*N. Samadani Langeroodi*

318

---

## Chemical Physics of Polymer Materials

Physicochemical Characteristics of the Radical Copolymerization of Fullerene-Containing Methacrylates with Vinyl Monomers

*Yu. N. Biglova, A. G. Mustafin, and M. S. Miftakhov*

324

The Role of Defective Structures of Butadiene-Nitrile Elastomers in Interphase Interactions in Mixtures with Ethylene-Propylene-Diene Rubbers

*N. M. Livanova and A. A. Popov*

330

On the Possibility of Regulating the Rate of Enzymatic Destruction of Chitosan in an Acetic Acid Solution

*V. V. Chernova, I. F. Tuktarova, and E. I. Kulish*

338

---

## Chemical Physics of Nanomaterials

Molecular Mechanism of the Spontaneous Segregation of Enantiomers in Liquid Nanoblobs

*D. V. Zlenko, M. A. Tregubova, and S. V. Stovbun*

343

Photoaccumulating Film Systems Based on  $\text{TiO}_2/\text{MoO}_3$  and  $\text{TiO}_2/\text{MoO}_3:\text{V}_2\text{O}_5$  Nanoheterostructures

*T. V. Sviridova, L. Yu. Sadovskaya, A. I. Kokorin, E. A. Konstantinova, V. E. Agabekov, and D. V. Sviridov*

348

Interaction of Pure and Metal Atom Substituted Carbon Nanocages with CNCl: a DFT Study

*Mohammad T. Baei, Mohammad Ramezani Taghartapeh, Alireza Soltani, Komail Hosseni Amirabadi, and Niloofar Gholami*

354

---

## Dynamics of Transport Processes

A DSC and NMR-Relaxation Study of the Molecular Mobility of Water Protons Interacting with Chemically Modified Starches

*A. I. Sergeev, N. G. Shilkina, L. A. Wasserman, S. I. Shilov, and H. Staroszczyk*

361

---

## Surface Reactions

Effect of the Electric Potential on the Interaction of Gold Nanoparticles Deposited on a Graphite Substrate with Molecular Hydrogen

*A. K. Gatin, M. V. Grishin, N. N. Kolchenko, S. Yu. Sarvadii, and B. R. Shub*

370

---

## Chemical Physics of Atmospheric Phenomena

Odd Oxygen and Its Atmospheric Lifetime

*I. K. Larin*

375

---