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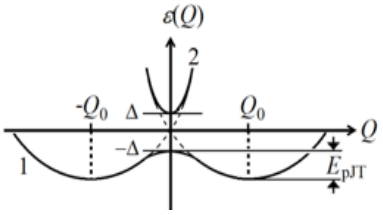
INVITED PAPER *PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS* 7

SPONTANEOUS SYMMETRY BREAKING AS A LAW OF NATURE
Isaac Bersuker

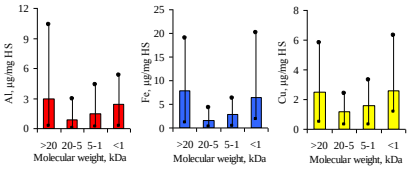
This paper discusses the notion of symmetry of polyatomic systems defined as invariance under transformations, and showes that this important property of atomic matter is extremely vulnerable, and may undergo internal breakdown, subject to the presence of electronic degeneracy or pseudodegeneracy. It is shown that electronic degeneracy and its extended form, called pseudodegeneracy, are actually the only source of spontaneous symmetry breaking (SSB) in nature, including all forms of matter, beginning with elementary particles, via nuclei, atoms, molecules, and solids. Theoretically, the vulnerability of the notion of symmetry is due to the fact that, following quantum mechanics, the separation of the motion of electrons and nuclei (and, similarly, the separation of motions of elementary particles) is approximate, and hence the classical notion of polyatomic space configuration is approximate too, with SSB as one of its main violation.



RESEARCH PAPER *ECOLOGICAL CHEMISTRY* 15

THE ROLE OF VARIOUS FRACTIONS OF HUMIC SUBSTANCES FROM SURFACE WATER IN BINDING Al(III), Fe(III), AND Cu(II) INTO COMPLEXES
Vladyslav Zhezherya, Petro Linnik, Rostyslav Linnik

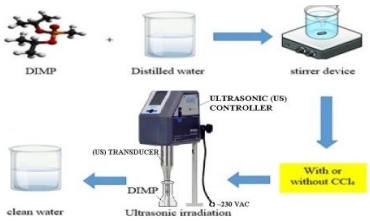
The aim of this research work was to evaluate the role of different fractions of humic substances in the binding of Al(III), Fe(III) and Cu(II) ions into complexes. The share of humic substances with a molecular weight of 20–5 kDa increases from 37% to 59%, when the total concentration of humic substances also increases. It was established that humic substances with molecular weight 20–5 kDa bounded the smallest amount of Al(III), Fe(III) and Cu(II) into complexes.



RESEARCH PAPER *ECOLOGICAL CHEMISTRY* 28

DEGRADATION OF DIISOPROPYL METHYLPHOSPHONATE IN AQUEOUS SOLUTIONS BY ULTRASONIC IRRADIATION
Muslim Hasan Allawi, Riyadh Sadeq ALMukhtar, Shurooq Talib Al-Humairi, Ali Dawood Salman, Tatjána Juzsakova, Viktor Sebestyén, Igor Cretescu

The degradation of diisopropyl methylphosphonate (DIMP) in aqueous solutions was studied using ultrasound irradiation with a fixed frequency of 26.6 kHz, following the first-order kinetic model. The experimental parameters, including the pH, the initial concentration of DIMP, the processing time, and the concentration of the additive CCl_4 were investigated. The best degradation efficiency of 98% was observed at pH of 10, adding 0.8 g/L CCl_4 for a processing time of 45 min.



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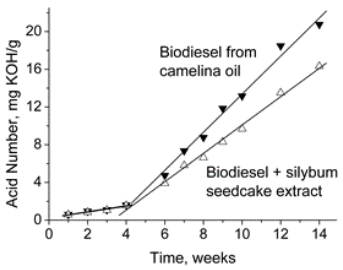
ANTIOXIDANT PROPERTIES OF SOME PLANT EXTRACTS AND EFFECT OF THEIR ADDITION ON THE OXIDATION STABILITY OF BIODIESEL
Pavlo Kuzema, Iryna Laguta, Oksana Stavinskaya, Viktor Anishchenko, Anastasiia Kramar, Natalia Smirnova, Tetiana Fesenko, Roman Ivannikov, Oksana Linnik

The extracts from the leaves of *Deschampsia antarctica*, *Camelina sativa*, and *Camellia japonica* plants, as well as from *Camelina sativa* and *Silybum marianum* seedcakes were investigated as potential additives for improvement of biodiesel stability against oxidation. In spite of significant distinctions in the content of various phenolic compounds, all the extracts were found to effectively inhibit DPPH radicals and decelerate transformation of fatty acid esters of biodiesel into organic acids by ~9-26%. Various extracts were shown to have different activity towards the biodiesel from rape and camelina seed oils; this result is consistent with the assumption that there is no universal stabilizer for different types of biodiesel.



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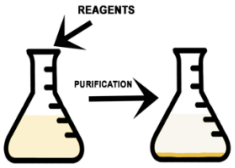
RESEARCH PAPER *INDUSTRIAL CHEMISTRY* 45

LOW WASTE TECHNOLOGY FOR MINE WATERS TREATMENT USING LIME AND ALUMINIUM COAGULANTS
Inna Trus, Vita Halysh, Mariia Tverdokhlib, Mukola Gomelya

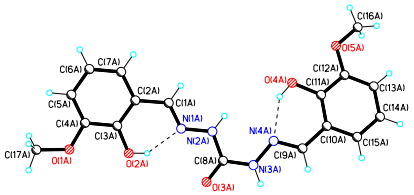
In this paper the process of reagent desalination of mineralized mine waters was studied. Reagents 5/6 aluminum hydroxochloride and sodium aluminate were used during liming. Complex processing of waste generated during reagent water treatment allows to create a low-waste technology for the purification of mineralized water.



RESEARCH PAPER *INORGANIC AND COORDINATION CHEMISTRY* 53

CRYSTAL STRUCTURE AND NMR SPECTROSCOPIC CHARACTERIZATION OF 1,5-BIS(2-HYDROXY-3-METHOXYBENZYLIDENE)CARBONOHYDRAZIDE
Natalia Talmaci, Diana Dragancea, Elena Gorincioi, Pavlina Bourosh, Victor Kravtsov

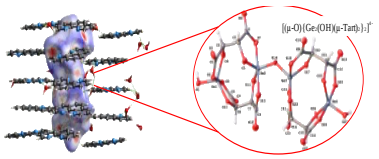
The crystal structure of 1,5-bis(2-hydroxy-3-methoxybenzylidene) carbonohydrazide was determined by X-ray single crystal diffraction study. In solid-state the molecule adopts the *anti* keto conformation, while NMR studies proved evidence on the presence of its *syn* tautomer in DMSO solution.



RESEARCH PAPER *INORGANIC AND COORDINATION CHEMISTRY* 61

SELECTIVITY, SYNTHESIS, CRYSTAL STRUCTURE AND BIOLOGICAL ACTIVITY OF THE ANION-COORDINATION PHENANTHROLINIUM TARTRATOGERMANATE
Eleonora Afanasenko, Inna Seifullina, Elena Martsinko, Viktoriya Dyakonenko, Svitlana Shishkina

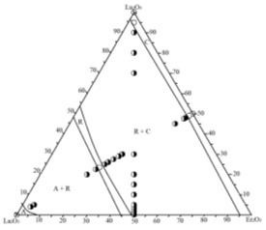
The present study extends the research and describes synthesis strategy, structural properties and biological activity of complex compound $(HPhen)_4[(\mu\text{-}O)\{Ge_2(OH)(\mu\text{-}Tart)_2\}_2]\cdot 9H_2O$, which comprises a tartratogermanate anion and the protonated form of 1,10-phenanthroline as the cationic component.



RESEARCH PAPER *PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS* 69

ISOTHERMAL SECTION OF THE La_2O_3-Lu_2O_3-Er_2O_3 TERNARY PHASE DIAGRAM AT 1250°C
Olga Chudinovych

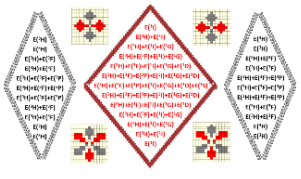
The isothermal section of the La_2O_3–Lu_2O_3–Er_2O_3 phase diagram at 1250°C has the characteristic three one-phase fields (A-La_2O_3, R, C-Lu_2O_3(Er_2O_3)) corresponding to solid solutions based on starting components and two two-phase fields (C + R, A + R) between them.



RESEARCH PAPER *PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS* 78

ON THE CALCULATION OF LANTHANIDE SYSTEMS. THE SPECTRAL PARAMETERS OF PRASEODYMIUM TRIVALENT ION
Ana Maria Toader, Maria Cristina Buta, Fanica Cimpoesu

The *ab initio* account of f and d electrons in lanthanide ions is assessed taking the Pr(III) ion. This shows rich experimental data and analytical tractability of spectral terms. The calculations are reaching a moderate match to experiment, the analysis identifying the actual impediments and suggesting ways of possible improvement.



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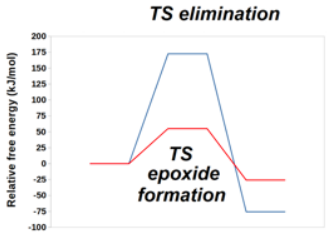
COMPUTATIONAL INSIGHTS INTO THE SPONTANEITY OF EPOXIDE FORMATION FROM HALOHYDRINS AND OTHER MECHANISTIC DETAILS OF WILLIAMSON'S ETHER SYNTHESIS
Pedro Silva

DFT computations identify the effects that enable the synthesis of geometrically-strained epoxide from deprotonated halohydrins. These computations also explain the preference for the formation of larger cyclic ethers with five-atom rings over six-atom-rings. Increased temperature favors elimination over S_N2 only when the reacting moieties are part of separate molecules.



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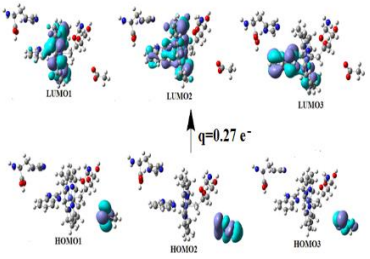
THE Co-N BOND CLEAVAGE IN THE ADENOSYNCOBALAMIN COFACTOR IN ADVANCE TO GLUTAMATE MUTASE AND METHYLMALONYL-CoA MUTASE PROCESSES
Tudor Spataru

The Pseudo-Jahn-Teller-Effect governs the glutamate mutase and methylmalonate-CoA mutase preliminary step and provides insight into particular details of *in vivo* C-N bond cleavage reactions of the adenosylcobalamin cofactor. Multi-configurational self-consistent field (MCSCF) calculations show that the preliminary step reaction glutamate mutase and methylmalonate-CoA mutase processes occur in the absence of total energy barriers.



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INSTRUCTIONS FOR AUTHORS