

CONTENTS

STRUCTURE OF BIOLOGICALLY ACTIVE COMPOUNDS

Theory of molecular structure and chemical bonding

- Nechaeva L.S., Butyrskaya E.V., Zapryagaev S.A.** Computer simulation of amino acid sorption on carbon nanotubes 233
- Ten G.N., Glukhova O.E., Slepchenkov M.M., Shcherbakova N.E., Baranov V.I.** Theoretical study of the mechanism of tautomeric transformations in the dimer of 7-azaindole and complex 7-azaindole with the water molecule by the methods of optical spectroscopy 242
- Fedorov M.S., Giricheva N.I.** Manifestation of Gauche Effect in benzenesulfonic acid hydrazide conformers 253
- Khaleghi-Rad A., Beyramabadi S.A., Morsali A., Ebrahimi M., Khorasandi-Chenarboo M.** Tautomerism of the antiepileptic drug Felbamate: A DFT study 261

Study of the structure of molecules by physical methods

- Tezcan H., Tokay N.** Structural and spectral properties of 3-substitutedphenyl-1,5-diphenylformazans: a quantum chemical study 269
- Pacheco A.G., Salgado-Morán G., Gerli-Candia L., Ramírez-Tagle R., Glossman-Mitnik D., Misra A., De Carvalho Alcântara A.F.** Theoretical investigation of the molecular structure and spectroscopic properties of oxicams 278

Structure of liquids and solutions

- Anikeenko A.V., Zelikman M.V., Kadtsyn E.D., Medvedev M.N.** Simulation of glycyrrhizic acid associates with cholesterol in methanol 285
- Gamov G.A., Aleksandriiskii V.V., Sharnin V.A.** Structure of pyridoxine solvates in an aqueous solution from quantum chemical calculations and NMR spectroscopy 293

Crystal chemistry

- Mironova E.V., Krivolapov D.B., Litvinov I.A., Mustakimova L.V., Mamedov V.A.** Structure of new derivatives of perhydropyrimidine-2-ones and intermolecular interactions in their crystals 300
- Adizov Sh.M., Tashkhodzhaev B., Kunafiev R.Zh., Mirzaeva M.M., Yuldashev P.Kh.** Crystal structure of pseudokopsinine and its salts 308
- Ahmad M., Perveen Z., Bortoluzzi A.J., Hameed S., Raza Shah M., Tariq M., Ud Din G., Anwar M.** Structural diversities and preliminary antimicrobial studies of 1-((*E*)-(pentylimino)methyl) naphthalen-2-ol and its metal complexes 314

Supramolecular compounds and nanosized systems

- Yakalı G., Öztürk S.E., Aygün M.** Strong hydrogen bonded supramolecular architecture in a crystal of the {3-[2-(1,3-benzodioxol-5-yl)-7-methoxy-1-benzofuran-5-yl] propyl} diethylamine cation with the hydrogen bonded chloride hydrate anion (halides) assembly: X-ray structure, dft calculations, hirshfeld surface analysis 321

Review

- Kurus N.N., Dultsev F.N.** Measurement of the unwinding force of a DNA double helix. 332

Brief communications

- Mitin A.V.** Mutual polarization of amino acids in small tetra-heme cytochrome *c* 1M1P. 357

Mahani M., Sheikghomi S., Sheikghomi H., Fasihi J. Quantitative structure activity relationship study on binding affinity of some aminothiazole derivatives with dopamine receptor in brain	361
Zha G.-J. Spin-Forbidden CO Binding to Iron—sulfur Cluster-free Hydrogenase: A Density Functional Study	366
Shmatko N.Yu., Korchagin D.V., Shilov G.V., Sanina N.A., Aldoshin S.M. Molecular and crystal structure of a cationic dinitrosyl iron complex with 1,3-dimethylthiourea	370
Slyvka Yu.I. Crystal structure of AgClO ₄ π -complex with 2-amino-5-allylthio-1,3,4-thiadiazole of [Ag(C ₅ H ₇ N ₃ S ₂)(ClO ₄)] composition	373
Popov L.D., Borodkin S.A., Tkachev V.V., Tupolova Yu.P., Burlov A.S., Shilov G.V., Utenyshev A.N. Crystal structure of copper(II) 2-methyl-3-{[3-methyl-5-oxo-1-phenylpyrazole-4-ylidene-methyl]amino}-quinazoline-4-onate	375
Mironova E.V., Krivolapov D.B., Litvinov I.A., Mustakimova L.V., Mamedov V.A. Molecular and crystal structure of 4-dichloromethylene-5-benzoyl-6-phenyl-perhydropyrimidin-2-one and its N(1)-substituted analogue	379
Popov L.D., Borodkin S.A., Tupolova Yu.P., Levchenkov S.I., Tkachev V.V., Burlov A.S., Tsaturyan A.A. Molecular and crystal structure of a novel Schiff base: 4-methyl-N-[2-[(2-methyl-4-oxo-quinazoline-3-yl)iminomethyl]phenyl]benzenesulfonamide	383
Jothi L., Anuradha G., Vasuki G., Ramesh Babu R., Ramamurthi K. Crystal structure of N-(<i>p</i> -methylbenzylidene)- <i>p</i> -bromoaniline	387

**PROCEEDINGS of the 17th Symposium on the intermolecular interaction
and molecular conformations: to the 100th anniversary of A.I. Kitaigorodsky,
June 23—27, 2014, Pushchino, Russia**

Grineva O.V. Analysis of aliphatic α,ω -diols crystal structures. Application and progress of A.I. Kitaigorodsky' ideas	390
Bogdan T.V., Alekseev E.S. Role of the conservative interhelical hydrogen bond SER74—TRP158 at the cholesterol binding site in the conformational stability of the β_2 -adrenergic receptor: molecular dynamics simulation	402
Paston S.V., Nikolaev A.I., Ushkov P.A. Complexes of EDTA, thymidine and Cu ²⁺ ions revealed by mass-spectrometry	410
Paston S.V., Polyanichko A.M., Shulenina O.V. Study of DNA interaction with Cu ²⁺ and Mg ²⁺ ions in the presence of caffeine	417
Kasyanenko N.A., Qiushi Z., Varshavskii M.S., Bakulev V.M., Demidov V.N. DNA metal complexes and metallization of a macromolecule in solution	424
Unksov I.N., Kasyanenko N.A. Conformational changes in the DNA molecule in solution caused by the binding of a light-sensitive cationic surfactant	431
Morozova E.A., Linkova N.S., Khavinson V.Kh., Soloviev A.Yu., Kasyanenko N.A. Interaction with peptide AEDL DNA <i>in vitro</i>	438