

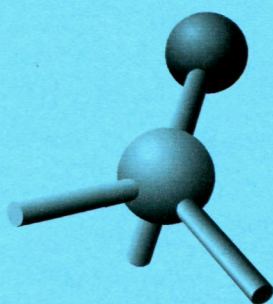


ISSN 0136-7463

РОССИЙСКАЯ АКАДЕМИЯ НАУК

Том 59  
Июнь  
Июль  
**2018**

# ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ



**№ 5**

НОВОСИБИРСК

ЖУРНАЛ  
СТРУКТУРНОЙ  
ХИМИИ

НАУЧНЫЙ ЖУРНАЛ

Основан в 1960 г.

Выходит 8 раз в год

Т О М 59

Июнь-июль

№ 5, 2018

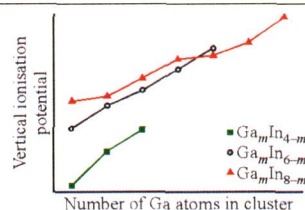
СОДЕРЖАНИЕ

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Hakkar F., Zouchoune B.

**Predicted structures and electronic properties of gallium-indium clusters  $Ga_mIn_{n-m}$  ( $n = 4, 6, 8$  and  $m < n$ ): A density functional study**

**Keywords:** relative stabilities, bonding interactions, ionization potential, electron affinity, chemical hardness



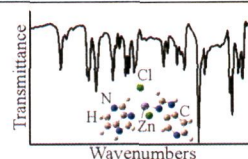
1043

ТЕОРИЯ СТРОЕНИЯ МОЛЕКУЛ И ХИМИЧЕСКОЙ СВЯЗИ

Badođlu S., Yurdakul Ş.

**Experimental and theoretical study on the new Zn(II) halide complexes of 3,5-diazaindole**

**Keywords:** 3,5-diazaindole, metal complexes, FTIR, NMR, DFT

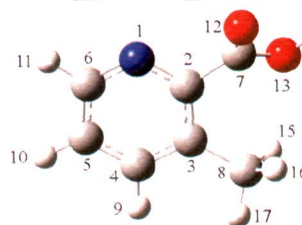


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Ramesh G., Prashanth J., Laxman Naik J., Venkatram Reddy B.

**Molecular structure, vibrational analysis, hyperpolarizability and NBO analysis of 3-methyl-picolinic acid using SQM calculations**

**Keywords:** methyl-picolinic acid, DFT, FTIR and FT-Raman spectra, vibrational analysis, dipole moment, hyperpolarizability, NLO effect, NBO analysis

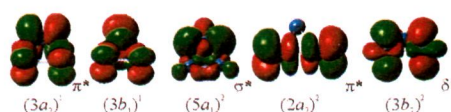


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Jin Q., Jin B., Zhang Z.-H., He X.-N.

**Aromaticity of the bare iridium trimers and  $Ir_3M^{0/+}$  and  $Ir_3M_2^{+/3+}$  ( $M = Li, Na, K$  and  $Be, Ca$ ) bimetallic clusters**

**Keywords:** iridium trimers, aromaticity, DFT calculation



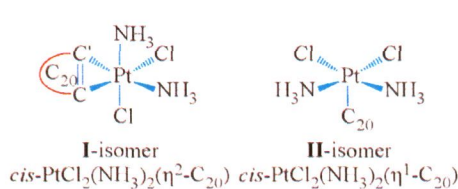
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Kazemi Z., Ghiasi R., Jamehbozorgi S.

**Analysis of the interaction between  $C_{20}$  cage and *cis*-PtCl<sub>2</sub>(NH<sub>3</sub>)<sub>2</sub>:**

**A DFT investigation of solvent effect, structures, properties and topologies**

**Keywords:**  $C_{20}$  cage, cisplatin, energy decomposition analysis (EDA), solvent effect, quantum theory of atoms in molecules (QTAIM)



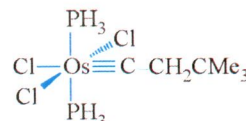
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**Exploring of solvent effects on the spectroscopic properties (IR and  $^{13}\text{C}$  NMR) in the  $\text{OsCl}_3(\equiv\text{CCH}_2\text{CMe}_3)(\text{PH}_3)_2$  carbyne complex**

**Keywords:** carbyne complex, Kirkwood–Bauer–Magat equation (KBM), solvent effect, linear solvation energy relationship (LSER)

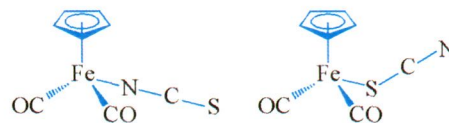


Fereidoni S., Ghiasi R., Pasdar H.

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**Theoretical study of solvent effect on the electronic and vibrational properties of  $[\text{CpFe}(\text{CO})_2(\text{NCS})]$  and  $[\text{CpFe}(\text{CO})_2(\text{SCN})]$  linkage isomers**

**Keyword:** linkage isomers, solvent effect, natural bond orbital analysis (NBO), Kirkwood–Bauer–Magat equation (KBM), energy decomposition analysis (EDA), Quantum theory of atoms in molecules analysis (QTAIM)

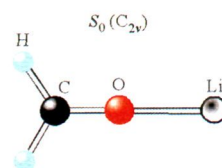


Shuai Z., Li A.Y.

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**Excited states of weak interacting complexes between formaldehyde and alkali metal ions**

**Keywords:** excited states, time-dependent density-functional theory (TD DFT), the  $\text{C}=\text{O}\cdots\text{M}^+$  interaction, infrared spectra, red shift and blue shift

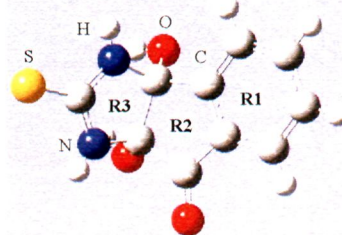


Hasan T., Ghalib R.M., Mehdi S.H., Singh P.K., Kumar A., Misra N.

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**Vibrational spectra, NBO and NLO analyses, and a molecular docking study of 3a,8a-dihydroxy-2-thioxo-1,3,3a,8a-tetrahydroindeno[1,2-d]imidazol-8(2H)-one using DFT**

**Keywords:** 3a,8a-dihydroxy-2-thioxo-1,3,3a,8a-tetrahydroindeno[1,2-d]imidazol-8(2H)-one, vibrational analysis, DFT, NLO, NBO, molecular docking

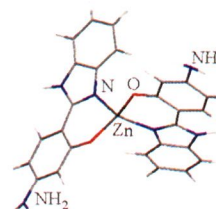


Tong Y.-P., Liu H., Lin Y.-W.

1130

**A density functional investigation of geometrical and electronic structure, charge transfer, and photoluminescent property of a zinc(II) complex with 5-amino-2-(1H-benzoimidazol-2-yl)-phenol**

**Keywords:** theoretical calculation, electronic structure, photoluminescence, LLCT, zinc(II)



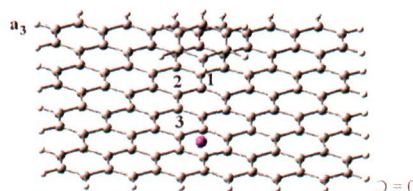
**ИССЛЕДОВАНИЕ СТРОЕНИЯ МОЛЕКУЛ ФИЗИЧЕСКИМИ МЕТОДАМИ**

Karimi P.

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**Investigation of simultaneous cation- $\pi$  and  $\pi$ - $\pi$  stacking interactions on graphene and some bent graphenes as curved surfaces of carbon nanohorns**

**Keywords:** bent graphene, carbon nanohorns, cation- $\pi$ ,  $\pi$ - $\pi$  stacking, aromaticity

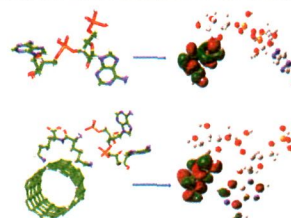


Yavari M., Beyramabadi A. S., Morsali A., Bozorgmehr M.R.

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**Tautomerization reaction, experimental and theoretical characterizations of the N,N'-dipyridoxyl(4-methyl-1,2-phenylenediamine) Schiff base and its Cu(II) complex**

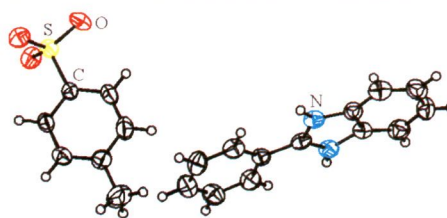
**Keywords:** synthesis, Schiff base, pyridoxal, DFT, copper, assignment, NBO, tautomerization



Sudhakar C., Saravanabhavan M., Sekar M., Babu B., Chandrasekaran J.

### Crystal structure and third order nonlinear optical studies on 2-phenylbenzimidazolium-*p*-toulenesulphonate

**Keywords:** 2-phenylbenzimidazolium-*p*-toulenesulphonate, nonlinear refractive index, absorption coefficient, third order nonlinear optical susceptibility



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Dehghanpour H.R.

### High coercivity induced in nickel ferrite nanoparticles by mechanical milling

**Keywords:** nickel ferrite, nanoparticle, combustion, coercivity

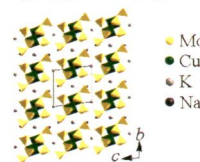


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Dridi W., Zid M.F.

### Crystal structure of new one-dimensional triple molybdate $\text{Na}_2\text{K}_2\text{Cu}(\text{MoO}_4)_3$

**Keywords:** solid state, X-ray diffraction, bond valence analysis, triple molybdate, charge distribution

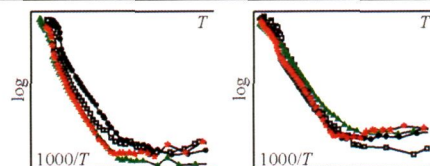


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Kıř M., Arı M., Polat Y., Erdođan B., Karaaslan T.

### Structural and temperature dependent electrical conductivity properties of $\text{Dy}_2\text{O}_3$ - $\text{Sm}_2\text{O}_3$ co-doped $\text{Bi}_2\text{O}_3$

**Keywords:** electrical conductivity, solid oxide fuel cell, solid state synthesis method, arrhenius equation, activation energy



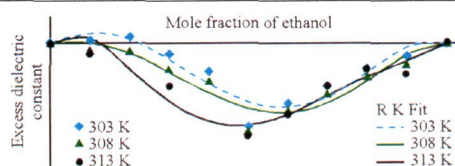
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## СТРУКТУРА ЖИДКОСТЕЙ И РАСТВОРОВ

Maharolkar A.P., Murugkar A., Khirade P., Mehrotra S.

### Temperature dependent microwave dielectric characterization of associated liquids

**Keywords:** density, viscosity, Bruggeman factor, excess inverse relaxation time, excess moalr polarization

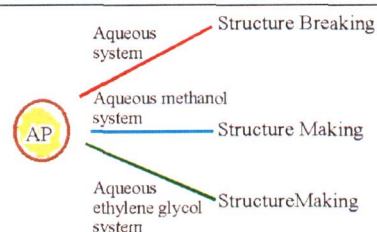


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Masood S., Rehman W., Khan Z., Arshad H., Begum S., Perveen A.

### Structure breaking/making property of acefylline piperazine in aqueous, aqueous methanol, and aqueous ethylene glycol systems

**Keywords:** density, acefylline piperazine, drug, methanol, ethylene glycol, structure breaking/making



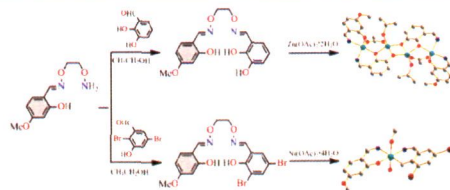
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## КРИСТАЛЛОХИМИЯ

Dong X.-Y., Du G.-M., Dong W.-K., An G.-X.

### Tetranuclear zinc(II) and mononuclear nickle(II) complexes based on asymmetrical salamo-type ligands: Syntheses, crystal structures, and fluorescence properties

**Keywords:** asymmetric Salamo-type ligand, transition metal complex, synthesis, crystal structure, spectroscopic behavior



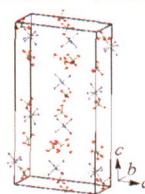
1198

Narulkar D.D., Srivastava A.K., Butcher R.J., Dhuri S.N.

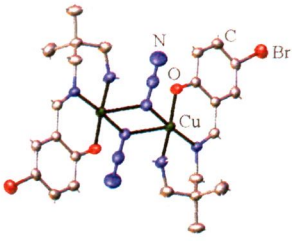
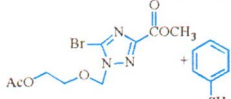
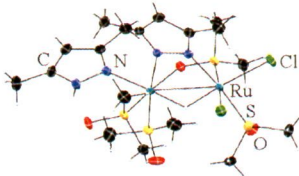
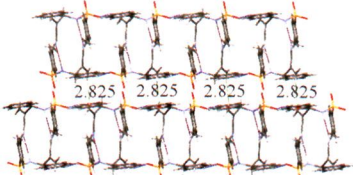
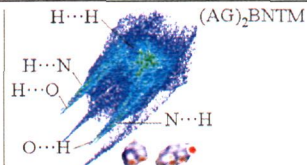
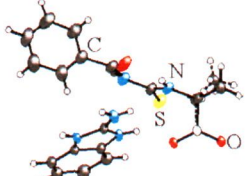
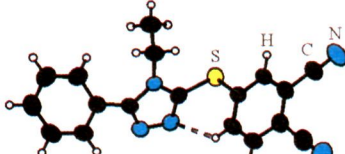
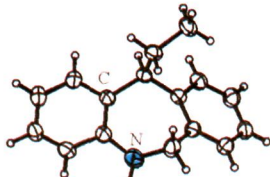
### Crystal structure of mononuclear non-heme nickel(II) octahedral complex:



**Keywords:** nickel(II), single crystal X-ray crystallography, bqenH<sub>2</sub>, 2,2'-bipyridine, hydrogen bonding, centrosymmetric, monoclinic



1208

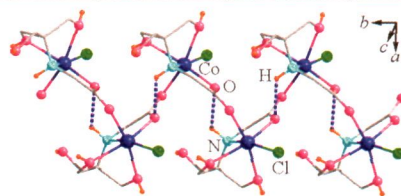
<p>Ghaemi A., Keyvani B., Fayyazi K., Rudbari H.A.</p> <p><b>Crystal structure of the azido-bridged copper(II) complex <math>[\text{Cu}_2\text{L}_2(\mu_{1,1}\text{-N}_3)_2]</math> based on the 2-[(3-amino-2,2-dimethylpropylimino)-methyl]-4-bromophenol Schiff base ligand</b></p> <p><b>Keywords:</b> synthesis, Schiff base ligand, copper(II), crystal structure, 2-[(3-amino-2,2-dimethylpropylimino)-methyl]-4-bromophenol, azido-bridged, X-ray diffraction analysis</p>	 <p>1216</p>
<p>Zhang D.-H., Duan Y.-P., Liu Y.</p> <p><b>Fluorescent chemosensor for <math>\text{Pb}^{2+}</math> based on 1,2,4-triazole</b></p> <p><b>Keywords:</b> synthesis, 2,4-triazole, fluorescence quenching, <math>\text{Pb}^{2+}</math></p>	 <p>1221</p>
<p>Kharbani D., Kurbah S.D., Rymmai E.K.</p> <p><b>Crystal structures of Ru(II) complexes with pyrazole and pyrazolate derivatives of tris(3,5-dimethylpyrazolyl)borohydride</b></p> <p><b>Keyword:</b> scorpionate degradation, pyrazole, pyrazolate-bridge, Ru(II)</p>	 <p>1226</p>
<p>Souza R.A.C., Guilardi S., Rubinger M.M.M., Terra L.R., Tavares E.C., Ellena J.A.</p> <p><b>Crystal structure of <i>N</i>-(2-cyano-1-phenylprop-2-en-1-yl)-4-methylbenzenesulfonamide</b></p> <p><b>Keywords:</b> synthesis, X-ray crystallographic analysis, allylsulfonamide, Morita-Baylis-Hillman adduct</p>	 <p>1232</p>
<p>Yin X., Wang J., Ma Q., Wang S.-M.</p> <p><b>Crystal structure and properties of bis (5-nitroimino-1,2,4-triazolate-3-yl) methane aminoguanidium salt</b></p> <p><b>Keywords:</b> nitrogen-rich salt, crystal structure, Hirshfeld surface, thermal stability</p>	 <p>1235</p>
<p>Odame F., Hosten E.C., Betz R., Lobb K., Tshentu Z.R.</p> <p><b>Characterization and computational studies of a co-crystal of 2-aminobenzimidazole and 2-[(benzoylcarbamoethioyl)amino]propanoic acid</b></p> <p><b>Keywords:</b> synthesis, alanine, amino acid, co-crystal, frontier orbitals</p>	 <p>1240</p>
<p>Ustabaş R., Çoruh U., Akçay H.T., Menteşe E., Vazquez-Lopez E.M.</p> <p><b>Crystal structure of 4-[(4-ethyl-5-phenyl-4H-1,2,4-triazol-3-yl)sulfanyl]phthalonitrile</b></p> <p><b>Keywords:</b> crystal structure, 1,2,4-triazol, phthalonitrile</p>	 <p>1245</p>
<p>Delgado G.E., Osal E., Mora A.J., González T., Palma A., Bahsas A.</p> <p><b>Structural characterization of 11-ethyl-6,11-dihydro-5H-dibenzo[b,e]azepine</b></p> <p><b>Keywords:</b> synthesis [b,e]dibenzazepine, amino-Claisen rearrangement, Friedel-Crafts, X-ray crystal structure</p>	 <p>1249</p>

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И НАНОРАЗМЕРНЫЕ СИСТЕМЫ

Zhou Y., Liu X., Hu L., Wang Q., Yao M., Song B.

**Solvothermal syntheses, crystal structure, and magnetic properties of a 1D Co(II) coordination polymer based on N-[tris(hydroxymethyl)methyl]glycine**

**Keywords:** cobalt(II), N-[tris(hydroxymethyl)methyl]glycine, magnetic properties

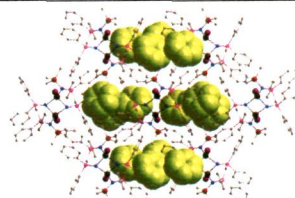


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Thirumoorthi R., Chivers T.

**Structural comparison of lithium iodide complexes of symmetrical and unsymmetrical [CH<sub>2</sub>(PPh<sub>2</sub>NSiMe<sub>3</sub>)(PPh<sub>2</sub>NR)](R = SiMe<sub>3</sub>, H) ligands**

**Keywords:** crystal structure, Si—N cleavage, iminophosphoranyl complexes, lithium iodide, Li<sub>2</sub>N<sub>2</sub> core

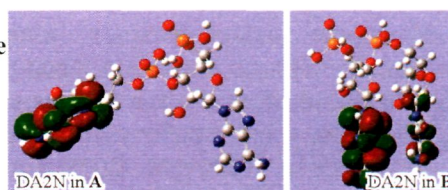


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Bagherolhashemi F., Bozorgmehr M.R., Momen-Heravi M.

**Biosensor properties of DA—DA dinucleotide in the presence of Di—L-lysine and single carbon nanotubes: Molecular dynamics simulation and density functional theory approach**

**Keywords:** diffusion coefficient, carbon nanotube, Fukui indices, HOMO, LUMO



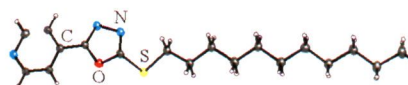
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СТРУКТУРА БИОЛОГИЧЕСКИ АКТИВНЫХ СИСТЕМ

Shen Z.-H., Wang Q., Sun Z.-H., Wu H.-K., Tan C.-X., Weng J.-Q., Liu X.-H.

**Crystal structure of 2-(pyridin-4-yl)-5-(undecylthio)-1,3,4-oxadiazole**

**Keywords:** heterocycle, synthesis, crystal structure

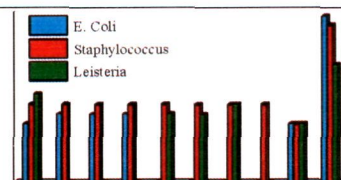


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Kantar C., Kaya B., Türk M., Şaşmaz S.

**Novel phthalocyanines containing guaiacol azo dyes: Synthesis, antioxidant, antibacterial and anticancer activity**

**Keywords:** phthalocyanine, azo dyes, antibacterial, antioxidant, anticancer



1280

Содержание следующего номера — в конце журнала