

Synthesis and Magnetism of Copper(II)–Ln(III)–Copper(II) (Ln = La, Nd, Eu, Gd, Tb, Dy, Ho, Er) Heterotrinary Complexes with N,N'-Bis(2-methyl-2-aminopropyl)oxamidocopper(II)

by Y.-T. Li¹, C.-W. Yan², S.-H. Wang³ and G.-L. Zhang¹

¹Marine Drug & Food Institute, Ocean University of China, 5 Yushan Road,
Qingdao, Shandong 266003, P. R. China

²Binzhou Vocational College, Binzhou, Shandong, 256624, P. R. China

³College of Marine Life Sciences, Ocean University of China, Qingdao, Shandong, 266003, P. R. China

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Eight new μ -oxamido-bridged copper(II)–lanthanide(III)–copper(II) heterotrinary complexes formulated as $\text{Cu}_2(\text{oxmap})_2\text{Ln}(\text{NO}_3)_3$ (Ln = La, Nd, Eu, Gd, Tb, Dy, Ho, Er), where oxmap stands for N,N'-bis(2-methyl-2-aminopropyl)oxamido dianions, have been synthesized by the strategy of “complex as ligand”, and characterized by elemental analyses, molar conductivity measurements, IR and electronic spectral studies. The variable temperature magnetic susceptibility (2~300 K), ESR measurements and studies of the $\text{Cu}_2(\text{oxmap})_2\text{Gd}(\text{NO}_3)_3$ complex have revealed that the central gadolinium(III) and terminal copper(II) ions are ferromagnetically coupled with the exchange integral $J_{(\text{Cu-Gd})} = +2.19 \text{ cm}^{-1}$, while an antiferromagnetic coupling is detected between the terminal copper(II) ions with the exchange integral $J'_{(\text{Cu-Cu})} = -0.15 \text{ cm}^{-1}$, on the basis of the spin Hamiltonian operator $[\hat{H} = -2J(\hat{S}_{\text{Cu1}} \cdot \hat{S}_{\text{Gd}} + \hat{S}_{\text{Cu2}} \cdot \hat{S}_{\text{Gd}}) - 2J'(\hat{S}_{\text{Cu1}} \cdot \hat{S}_{\text{Cu2}})]$. A plausible mechanism for the ferromagnetic coupling between copper(II) and gadolinium(III) is discussed in terms of spin polarization.

Key words: oxamido-bridge, copper(II), lanthanide(III), magnetism, heterotrinary complexes

Characterization of Cu_xS Layers Obtained by Adsorption–Diffusion Method on Polycapraamide from $\text{K}_2\text{S}_5\text{O}_6$ Solutions

by V. Krylova and N. Dukštienė

Faculty of Chemical Technology, Kaunas University of Technology,
Radvilenu str. 19, LT-50254 Kaunas, Lithuania

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Cu_xS layers on polycapraamide, obtained by the adsorption–diffusion method, have been studied. These layers are formed when the ions of pentathionate ($\text{K}_2\text{S}_5\text{O}_6$) sorbed into polycapraamide react with a solution of copper(I) salt. By X-ray diffraction studies it was determined that the Cu_xS layers obtained are of three phases, comprising *covellite* (CuS), *geerite* ($\text{Cu}_{1.6}\text{S}$), *anilite* ($\text{Cu}_{1.75}\text{S}$) and *chalcocite* (Cu_2S). The concentration ratio of the phases depends on the period of polycapraamide sulfuration in a potassium pentathionate solution. *Chalcocite* prevails in the composition of Cu_xS film on PKA. The films were characterized by means of IR spectroscopy. IR absorption spectra were investigated in the region of the wavenumbers $200\text{--}1400\text{ cm}^{-1}$. The characteristic absorption maxima were found in the regions $242\text{--}243$, $268\text{--}290$, $339\text{--}384$, $422\text{--}463$, 538 , $611\text{--}612$, $879\text{--}929$, $1018\text{--}1095$, $1186\text{--}1224\text{ cm}^{-1}$ and assigned, respectively, to $\delta(\text{S--S--S})$ and $\nu(\text{Cu--S})$, $\gamma_r(\text{SO}_3)$, $\nu(\text{S--S})$ and $\nu(\text{Cu--S})$, $\delta_{\text{as}}(\text{O--S--O})$, $\delta_{\text{s}}(\text{O--S--O})$, $\nu(\text{Cu--S})$, $\nu_{\text{s}}(\text{S--O})$ and $\nu_{\text{as}}(\text{S--O})$. Measurements of electrode potentials in CuSO_4 solutions of different concentration have shown that the response time and stability of electrodes in Cu^{2+} ion solutions depend on the phase composition. Electrodes composed from $\text{Cu}_{1.75}\text{S}$ and $\text{Cu}_{1.6}\text{S}$ are not stable in CuSO_4 solutions. The response time of a Cu_2S electrode depends on concentration change. The change of the potential with an active Cu^{2+} ion concentration is linear in the range of $1 \cdot 10^{-3}\text{--}4 \cdot 10^{-2}\text{ mol}\cdot\text{dm}^{-3}$, the slope of the linear portion being 31.5 mV per decade. The obtained experimental values have been compared with the theoretical values calculated on the basis of thermodynamic data.

Key words: polycapraamide, potassium pentathionate, sulfuration, diffusion, copper sulfide films

Template Synthesis of 16-Membered Octaazamacrocyclic Complexes of Fe(II), Co(II), Ni(II), Cu(II) and Zn(II) Ions

by T.A. Khan, S.S. Ghani and S. Tabassum

*Division of Inorganic Chemistry, Department of Chemistry,
Aligarh Muslim University, Aligarh – 202002, India*

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Template condensation of the metal ions with hydrazine, 2,4-pentanedione and acetaldehyde in a 1:4:2:2 molar ratio resulted in the formation of a new series of 16-membered octaazamacrocyclic complexes: dichloro/nitrato [2,5,8,10,13,16-hexamethyl-3,4,6,7,11,12,14,15-octaazacyclohexadecane-2,7,10,15-tetraene)metal(II)], [MLX₂] (M = Fe(II), Co(II), Ni(II), Cu(II) and Zn(II); X = Cl or NO₃). The overall geometry and stereochemistry of the complexes have been characterized by elemental analyses, IR, ¹H NMR, EPR, UV visible, magnetic susceptibility and conductivity measurements. An octahedral geometry is suggested for all of the complexes. The conductivity data suggest that the complexes are non-ionic in nature.

Key words: template synthesis, octaazamacrocycles, octahedral complexes, spectroscopic studies

Synthesis, Crystal Structures and Antibacterial Activities of a Pair of Isostructural Dinuclear Schiff Base Nickel(II) and Copper(II) Complexes

by Y.-X. Sun¹, D.-S. Kong¹, G. Yang² and Z.-L. You³

¹*Department of Chemistry, Qufu Normal University, Qufu 273165, P. R. China*

²*Department of Capital Management, Qufu Normal University, Qufu 273165, P. R. China*

³*Department of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, P. R. China*

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Two novel dinuclear Schiff base complexes, $[\text{Ni}_2\text{L}_2(\text{NCS})_2]$ (1) and $[\text{Cu}_2\text{L}_2(\text{NCS})_2]$ (2), where $\text{L} = 2\text{-}[(2\text{-dimethylaminoethylimino)methyl}]$ phenolate, have been synthesized and characterized by elemental analyses, IR, and single crystal X-ray diffraction. They are structurally similar. Each of the two metal ions of the complex is coordinated by two nitrogen and two oxygen atoms in the basal plane of a distorted square pyramid and by one nitrogen atom in its apex. The oxygen atoms belong to two Schiff base ligands and form bridges between two metal ions, while the nitrogen atoms of the basal plane belong to one ligand coordinated to a given metal atom. The apex nitrogen is that of the thiocyanate anion. The Schiff base and the two complexes showed effective antibacterial activities. It is noteworthy that the two complexes have stronger antibacterial activities than that of the corresponding Schiff base ligand.

Key words: Schiff base, complexes, crystal structure, antibacterial activity

Synthesis, Crystal Structure and Properties of Transition Metal-Azide Compounds with Bis(pyrazol-1-yl)methane

by L. Zhang¹, H.-Y. Gao², Y.-Y. Ge¹, F. Peng¹ and H. Xue²

¹Department of Chemical Engineering, South China University of Technology, Guangzhou 510640, P. R. China

²Department of Chemical Engineering, Guangxi University, Nanning 530004, P. R. China

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Two new compounds, $\text{Co}(\text{bpm})_2(\text{N}_3)_2$ (**1**) and $\{[\text{Ni}(\text{bpm})_2(\text{H}_2\text{O})_2][\text{Ni}(\text{bpm})_2(\text{N}_3)_2]\}(\text{ClO}_4)_2$ (**2**), where bpm refers to bis(pyrazol-1-yl)methane, have been prepared and characterized by elemental analyses, IR, UV-Vis spectra and X-ray diffraction. Crystal data for **1**: monoclinic, space group $\text{P}2_1/\text{n}$ with $a = 10.394(4)$, $b = 14.410(5)$, $c = 12.591(4)$ Å, $\beta = 91.194(7)^\circ$, $V = 1885.6(11)$ Å³ and $Z = 4$. Crystal data for **2**: triclinic, space group $\text{P}\bar{1}$ with $a = 8.7673(6)$, $b = 8.9618(6)$, $c = 13.5653(9)$ Å, $\alpha = 84.6040(10)^\circ$, $\beta = 84.4230(10)^\circ$, $\gamma = 79.6040(10)^\circ$, $V = 1040.19(12)$ Å³ and $Z = 1$. Complex **1** is a neutral monomer molecule, in which Co^{II} ion is coordinated by four nitrogen atoms from two chelating bpm and two terminal azide ligands to form a *cis*-octahedral configuration. However, compound **2** is composed of a neutral $[\text{Ni}(\text{bpm})_2(\text{N}_3)_2]$ entity, one $[\text{Ni}(\text{bpm})_2(\text{H}_2\text{O})_2]^{2+}$ cation and perchlorate anions, in which the neutral $\text{Ni}(\text{bpm})_2(\text{N}_3)_2$ entity is in a *trans*-six-coordinated configuration. The uncoordinated terminal nitrogen atom of azide forms O–H...N hydrogen bonds with the coordinated H_2O molecule to afford a one-dimensional chain structure.

Key words: crystal structure, azide, one-dimensional chain, hydrogen bond

The Thermodynamic Studies of the Molecular Interactions of Diphenyltin(IV) Dichloride and Dibromide with *meso*-Tetraarylporphyrins

by A. Zabardasti¹, M. Salehnassaje², M. Asadi³ and V.A. Karimivand³

¹Department of Chemistry, College of Sciences, Lorestan University, Khoramabad, I.R. Iran

²Ministry of Education, Zeinabieh High School, Khoramabad, I.R. Iran

³Department of Chemistry, College of Sciences, Shiraz University, Shiraz, I.R. Iran

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The thermodynamic parameters for interactions of Ph_2SnCl_2 and Ph_2SnBr_2 with *para*-substituted *meso*-tetraphenylporphyrins ($\text{H}_2\text{T}(4\text{-X})\text{PP}$; X = OCH_3 , CH_3 , H, Cl) have been studied. The formation constants have been calculated using UV-Vis titration spectra and computer SQUAD program. The adducts show the composition 2:1 of Ph_2SnX_2 to porphyrin. Formation constants decreased with decreasing electron donation of porphyrins and with decreasing electron withdrawing property of X group on the diphenyltin compound, as follow: $\text{H}_2\text{T}(4\text{-OCH}_3)\text{PP} > \text{H}_2\text{T}(4\text{-CH}_3)\text{PP} > \text{H}_2\text{TTPP} > \text{H}_2\text{T}(4\text{-Cl})\text{PP}$; and $\text{Ph}_2\text{SnCl}_2 > \text{Ph}_2\text{SnBr}_2$.

Key words: porphyrins, diphenyltin(IV) dihalide, diorganotin(IV) dihalide adducts, Siting-Atop type complexes

Iridoid Glucoside and Aryl Ester from *Buddleja crispa*

by I. Ahmad¹, A. Malik¹, N. Afza², I. Fatima¹, R.B. Tareen³,
S.A. Nawaz¹ and M.I. Choudhary¹

¹International Center for Chemical Sciences, HEJ Research Institute of Chemistry,
University of Karachi, Karachi-75270, Pakistan

²Pharmaceutical Research Centre, PCSIR Labs. Complex, Karachi-75280, Pakistan

³Department of Botany, University of Baluchistan, Pakistan

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Iridoid glucoside (**1**) and aryl ester (**2**) have been isolated from *Buddleja crispa* along with buddlejosides A₂ (**3**) and A₅ (**4**) isolated for the first time from this species. The structures of all of the compounds were determined by spectroscopic techniques and chemical studies. Compound **1** displayed lipoxygenase inhibitory potential with an *IC*₅₀ value of 52.5 ± 0.03 μM while compound **2** inhibited acetylcholinesterase and butyrylcholinesterase enzymes with *IC*₅₀ values of 36.5 ± 0.03 μM and 12.5 ± 0.02 μM, respectively.

Key words: *Buddleja crispa*, Buddlejaceae, iridoid glucoside, aryl ester, enzyme inhibition

**Synthesis and Properties of Azoles and Their Derivatives.
Part LVI. Mechanistic Aspects on the [2+3] Cycloaddition
of Z-C,N-Diphenylnitrone with *trans*-1-Nitropropene-1
and *trans*-3,3,3-Trichloro-1-nitropropene-1**

by **R. Jasiński** and **A. Barański**

*Institute of Organic Chemistry and Technology, Cracow University of Technology,
ul. Warszawska 24, 31-155 Cracow, Poland*

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The [2+3] cycloaddition reactions of diphenylnitrone with *trans*-1-nitropropene-1 and *trans*-3,3,3-trichloro-1-nitropropene-1 occur *via* a concerted mechanism despite high π -deficient character of dipolarophiles. This mechanism is indicated by *cis*-stereospecificity of the cycloaddition, the obtained values of activation parameters and weak solvent effect on the reaction kinetics.

Key words: [2+3] cycloaddition, nitrone, nitroalkenes, mechanism, kinetics

**Synthesis of Novel
4-Chloro-5-methyl-2-(R-thio)-N-(2,3-dihydro-1,3,4-
thiadiazol-2-ylidene)benzenesulfonamide Derivatives**

by **J. Sławiński**

*Department of Chemical Technology of Drugs, Medical University of Gdańsk,
Al. Gen. J. Hallera 107, 80-416 Gdańsk, Poland*

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Two series of novel 4-chloro-5-methyl-2-(R-thio)-N-(2,3-dihydro-1,3,4-thiadiazol-2-ylidene)benzenesulfonamide derivatives **5–14** were synthesized by the reaction of potassium 6-chloro-1,1-dioxo-7-methyl-1,4,2-benzodithiazine-3-thiolate (**1**) or 6-chloro-3-mercapto-7-methyl-1,4,2-benzodithiazine 1,1-dioxide (**2**) with hydrazonyl bromides **3a–g**. Suggested mechanisms of the investigated reaction were discussed. The molecular orbital calculation of the possible tautomeric forms of 3-mercaptobenzodithiazine **2** were also presented.

Key words: 4-chloro-5-methyl-2-(R-thio)-N-(2,3-dihydro-1,3,4-thiadiazol-2-ylidene)benzenesulfonamides, synthesis

Synthesis of New Quaternary Ammonium Salts – Derivatives of Phenyl Glucopyranosides

by B. Dmochowska¹, L. Pellowska-Januszek¹, E. Skorupa¹, A. Nowacki¹,
F. Stock², P. Stepnowski¹ and A. Wiśniewski¹

¹Department of Chemistry, University of Gdańsk, ul. Sobieskiego 18, PL-80-952 Gdańsk, Poland

²Centre for Environmental Research and Technology, University of Bremen,
Leobenerstr. 1, Bremen, Germany

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A new series of quaternary ammonium tosylates – derivatives of phenyl β -D-glucopyranoside – has been produced in reactions of phenyl 2,3,4-tri-*O*-acetyl-6-*O*-tosyl- β -D-glucopyranoside with triethylamine, trimethylamine, 4-(*N,N*-dimethylamino)pyridine, 2-methylpyridine and pyridine. The structures of the isolates were determined by spectral analysis, including extensive 2D NMR spectral analyses.

Key words: quaternary ammonium salt, phenyl glucopyranoside, tosylate, ¹H, ¹³C NMR

The Influence of Li Substitution on the Structure, Electrical and Magnetic Properties of La/BaCoO_{3-δ}

by M.Sh. Khalil and A.M. El-Sayed

Inorganic Chemistry Department, National Research Centre, Dokki, Cairo 12622, Egypt

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The influence of substitution of Co by lithium on the structural, electrical conductivity and magnetic properties of La_{0.7}Ba_{0.3}Co_{1-x}Li_xO_{3-δ} (x = 0.0 and 0.1) systems was investigated. Samples were prepared by the polymerized complex sol-gel technique and sintered at 900°C for 2 h. Thermal, XRD, and IR studies of the two systems confirm complete solid solution formation and crystallization with cubic perovskite structure. By replacing Co by Li (x = 0.1), the lattice parameter increases, and nanocrystalline particles in the range of 25–90 nm were obtained. The system with Li substitution has a higher electrical conductivity with lower activation energy and has a ferromagnetic behavior in the range of measuring temperatures and magnetic field.

Key words: La/BaCo/LiO₃, polymerized complex route, characterization, electrical conductivity, magnetic susceptibility

**A Hexanuclear Iodoargentate(I) Cluster of the Coplanar
Dicubane-like Type: Structure and Nonlinear Optical
(NLO) Properties of $\{[(t\text{-Bu})_4\text{N}]_2[\text{Ag}_6\text{I}_8]\}_n$**

by Y. Li¹, Z.X. Zhang¹, K.C. Li², W.D. Song¹, F. Huang¹, S.D. Li¹, X.W. Li¹,
J.Q. Xu² and L.Y. Pan³

¹*College of Science, Guangdong Ocean University, Zhanjiang 524088, P. R. China*

²*College of Chemistry, Jilin University, ChangChun 130023, P. R. China*

³*College of Physics, Jilin University, Changchun 130023, P. R. China*

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A polynuclear silver(I) complex $\{[(t\text{-Bu})_4\text{N}]_2[\text{Ag}_6\text{I}_8]\}_n$ **1** with iodo-bridging ligands has been prepared, the centrosymmetric cluster anion can be described as two $[\text{Ag}_4\text{I}_4]$ distorted cubane units sharing one $[\text{Ag}_2\text{I}_2]$ plane. This cluster polymer shows strong third-order nonlinear optical (NLO) absorption and refraction with absorption coefficient $\alpha_2 = 8.9 \times 10^{-10} \text{ m}\cdot\text{w}^{-1}$ and refractive index $n_2 = -6.6 \times 10^{-17} \text{ m}^2\cdot\text{w}^{-1}$.

Key words: iodoargentate(I) cluster, dicubane-like, structure, nonlinear optical properties

Compressibility Data and Virial Coefficients for Nitrogen-Argon Mixtures

by Ö. Korfali

*Faculty of Engineering and Technology, Galatasaray University,
Çırağan Caddesi, No: 36, Ortaköy 34357, Istanbul, Turkey*

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We present a detailed experimental study of the pressure and density of N₂-Ar mixtures at 0°C, 25.0°C and 50.0°C with four different mixtures at each temperature. The pressures are measured with a dead-weight tester. The densities are determined from knowledge of the precise volume and weight measurement of the mixtures. Statistical analysis of the experimental data yielded very precise values for the second and third density virial coefficients. Finally experimentally determined virial coefficients are compared with those calculated on the basis of statistical mechanics. The maximum percentage deviation between experimental and theoretical second virial coefficients is about 10% and that between third virial coefficients is less than 1%.

Key words: N₂-Ar mixtures, second virial coefficient, third virial coefficient

Spectrokinetic Study of the Reaction System of $2\text{NO}_2 \leftrightarrow \text{N}_2\text{O}_4$ with Some Fluorinated Derivatives of Ethanol and Propanols Between 293–358 K in the Gas Phase

by D. Wójcik-Pastuszka, I. Golonka and E. Ratajczak

*Department of Physical Chemistry, Wrocław Medical University,
Pl. Nankiera 1, 50-140 Wrocław, Poland*

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The gas phase kinetics of the reversible reactions between nitrogen tetroxide and some fluorinated alcohols in the reaction system $2\text{NO}_2 \leftrightarrow \text{N}_2\text{O}_4$ (1, 2) $\text{N}_2\text{O}_4 + \text{ROH} \leftrightarrow \text{RONO} + \text{HNO}_3$ (3, 4) have been studied by UV-Vis spectrophotometry to follow the NO_2 decay. The products – RONO (R = CH_2FCH_2 , CHF_2CH_2 , CF_3CH_2 , $\text{CHF}_2\text{CF}_2\text{CH}_2$, $\text{CF}_3\text{CF}_2\text{CH}_2$, CF_3CHCF_3) – were identified by their UV spectra and the values of the maxima UV absorption cross sections were determined in the range 320–400 nm. The rate constants for the forward reaction are $10^{-19}k_3^{\text{av}}/\text{cm}^3\text{molec}^{-1}\text{s}^{-1}$ 9.7±1.5; 2.5±0.4; 1.8±0.3; 23±3.5, 2.3±0.3, 0.2±0.03 and for the reverse reaction $10^{-19}k_4^{\text{av}}/\text{cm}^3\text{molec}^{-1}\text{s}^{-1}$ 4.6±0.7; 5.5±0.8; 4.9±0.7; 9.1±1.4; 7.7±1.2; 23±3.5 at 298 K for the reaction with 2-fluoroethanol, 2,2-difluoroethanol, 2,2,2-trifluoroethanol, 2,2,3,3-tetrafluoro-1-propanol, 2,2,3,3,3-pentafluoro-1-propanol and 1,1,1,3,3,3-hexafluoro-2-propanol, respectively, were derived by the computer simulation of monitored NO_2 decay profiles. The temperature dependence of the bimolecular rate constants k_3 and k_4 were studied in the temperature range 293–358 K and the activation energy for the forward E_3 and for the reverse E_4 reaction were derived. From the observed temperature dependence of the equilibrium constants $K_{3,4}$, expressed in terms of the van't Hoff equation, the thermochemical parameters for all reactions studied were estimated.

Key words: nitrogen dioxide, dinitrogen tetroxide, fluorinated alcohols

Liquid-liquid Distribution of Selected Derivatives of Benzoic Acid in 1-Octanol–Toluene–Water Systems

by **B. Papciak and S. Kopacz**

*Department of Inorganic and Analytical Chemistry, Chemical Faculty,
Rzeszów University of Technology, al. Powstańców Warszawy 6, 35-959 Rzeszów, Poland*

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The influence of 1-octanol on liquid-liquid distribution of chloro and methoxy derivatives of benzoic acid in toluene–water systems was presented. The values of partition constant (K_p) and dimerization constant (K_d) of investigated acids were calculated. It was found that raising of 1-octanol concentration in the mixture with toluene increases partition constants and decreases dimerization constants of the carboxylic acid.

Key words: liquid-liquid equilibria, carboxylic acid, partition constant, dimerization constant

Effect of the Dielectric Medium on the Conformational Behaviour of Methyl 3-Nitrobenzoate

by **A. Konopacka, J. Kalenik and Z. Pawełka**

Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland

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Conformational analyses of methyl 3-nitrobenzoate (**MNB**) was performed, employing DFT, MP2, and semi-empirical quantum-chemical calculations, as well as classical methods based on atomic charge and dipole moment approximations. Properties such as the relative energies of the O-NO₂ *trans* and O-NO₂ *cis* isomers, their populations and dipole moments, all in vacuum, were considered first. Then the conformational *trans* \rightleftharpoons *cis* equilibrium was quantitatively established by dipole moment measurements in solvents of dielectric permittivities between 2.016 and 10.34. Different approaches, based on continuum-dielectric and MSA models were explored to explain the contribution of the electrostatic interaction to the standard Gibbs energy change ΔG° of the *trans* \rightleftharpoons *cis* transformation in **MNB** in solution.

Key words: methyl 3-nitrobenzoate, rotational isomerism, theoretical calculations, dipole moment, electrostatic interaction, solvent effect