Critical Behavior Studies of 2,4-Dichlorobenzoic Acid – Amines Hydrogen-Bonded Complexes Utilizing Fourier-Transform Infrared Spectroscopy

by M.M. Habeeb

Chemistry Department, Faculty of Education, Alexandria University, Alexandria, Egypt

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A series of crystalline 1:1 hydrogen-bonded complexes between 2,4-dichlorobenzoic acid (DCBA) and various quinolines and pyridines was prepared. Fourier-transform infrared spectra (FTIR) of these complexes are presented and analyzed in the $\nu_{\text{OH}}$ and $\nu_{\text{C=O}}$ regions. The correlation between the gravity center of the protonic vibrations $v_{cg}$ (cm$^{-1}$), the quantity $\Delta v/\Delta v_{\nu}$, and the pK$_a$ values of the amines are presented. The integrated intensities in solution A (L mol$^{-1}$ cm$^{-2}$) and in the crystalline state A (kg mol$^{-1}$ cm$^{-2}$) in the $\nu_{\text{C=O}}$ region were correlated with the pK$_a$ values of the investigated amines. Striking anomalies are observed at the critical region (50% proton transfer). These results can be interpreted by assuming that quasi-symmetrical O..H..N bridge is formed with a single, flat minimum potential in the solid state and a double minimum potential in solution.
Spectrochemical Properties of Noncubic Transition Metal Complexes in Solutions. XIII. Angular Overlap Treatment of Diaquabis(salicylideneaminothiazole)cobalt(II)

by I. Kuźniarska-Biernacka and K. Kurzak

Department of Chemistry, University of Podlasie, PL 08-110 Siedlce, Poland

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Mixed ligand cobalt(II) complex with monodentate (water) and bidentate (Schiff base: salicylidene-2-aminothiazole) ligands has been characterized by elemental analyses, molar conductivities, ultraviolet (UV) and visible (VIS) spectroscopy. The electronic spectra of solids as well as solutions exhibit pseudo-octahedral coordination geometry for the cobalt centre. The molar conductivities indicate their non-electrolytic properties in solvents studied. Combined multi-technique experiments have been used to postulate the $C_2h$ geometry for the species in solutions and to determine the coordination properties of ligators and their bonding abilities (ligand-field parameters).
Kinetic, Spectroscopic and Magnetic Properties of 1,4,8,11-Tetraazacyclotetradecanenickel Bi- and Trivalent Complexes

by B. Banaś, M. Nahorska, B. Korybut-Daszkiewicz and J. Mroziński

1Faculty of Chemistry, University of Wrocław, F. Joliot-Curie 14, 50-383 Wrocław, Poland
2Institute of Organic Chemistry, Polish Academy of Sciences, M. Kasprzaka 44, 01-224 Warszawa, Poland
*jmroz@wchuwr.chem.uni.wroc.pl

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Nickel(II) and nickel(III) complexes of formula [NiLCl2] and [NiIIILCl2]+ containing tetraaza macrocyclic ligands with nitrogen donor atoms, where \( L = [14]aneN_4 \) (\( L^1 \)), 2-Me[14]aneN_4 (\( L^2 \)), 5,12-Me_2[14]aneN_4 (\( L^3 \)), 5,7,7,12,14,14-Me_6[14]aneN_4 (\( L^4 \)), form stable crystals with a pseudo-octahedral geometry of central atom. This work concerns the methyl analogues of Ni(II) and Ni(III) complexes. Magnetic and spectroscopic measurements gave values of spectroscopic parameter \( g \) and paramagnetic temperature dependence characteristic for this type of compounds. Their properties were investigated using EPR, reflectance spectroscopy and IR techniques. The Faraday method was used for the investigation of magnetic susceptibility between 4.2–300 K.
Predominance of Amino-Sulfonyl Hydrogen Bonding in (Z)-2-Benzene-sulfonyl-1-phenyl-2-(phenylhydrazono)ethanones in Crystals and in Solution: An Experimental NMR and X-ray Crystallographic and Theoretical Ab Initio and DFT/GIAO Studies

by E. Kolehmainen¹, A. Zakrzewski², A. Zakrzewska², M. Nissinen¹, B. Ośmia³owski² and R. Gawinecki²

¹Department of Chemistry, University of Jyväskylä, P.O. Box 35, FIN-40351 Jyväskylä, Finland
²Department of Chemistry, Technical and Agricultural University, Seminaryjna 3, PL-85-326 Bydgoszcz, Poland

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¹H, ¹³C, and ¹⁵N NMR spectra show that (Z)-2-benzenesulfonyl-1-phenyl-2-(phenylhydrazono)ethanone is the only tautomeric form detected in chloroform solution. Substituent in the phenylhydrazone moiety does not affect this tautomeric preference. Ab initio calculations show that (Z)-2-benzenesulfonyl-1-phenyl-2-(phenylhydrazono)ethanone is really favoured over its proton transfer products in chloroform solution. This shows that N-H...OS(O) interaction is much stronger than the hydrogen bonds in other tautomeric forms. The (Z)-2-benzenesulfonyl-1-phenyl-2-(phenylhydrazono)ethanone tautomer was also detected in the crystal state.
New Method for the Synthesis of Azocrown Compounds Containing Oxygen, Nitrogen and Oxygen, or Sulfur Atoms in the Macroring

by E. Luboch and A. Biedrzycka

Department of Chemical Technology, Technical University of Gdańsk,
Narutowicza 11/12, 80-952 Gdańsk, Poland
E-mail: elub@chem.pg.gda.pl

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A new method for the synthesis of azocrown ethers with different heteroatoms in macrocycle and of different size of molecular hole has been described. This method consists in reaction of 2,2'-difluorozobenzene with diols, diamine, aminodiol and dithiol in the presence of base.
Syntheses of a New Series of N-Amino-N′-(benzenesulphonyl)guanidine Derivatives with Potential Antitumor Activity

by J. Sławiński1, P. Bednarski2, R. Grüner2 and P. Reszka2,3

1Department of Chemical Technology of Drugs, Medical University of Gdańsk, Al. Gen. J. Hallera 107, 80-416 Gdańsk, Poland; E-mail: jaroslaw@farmacja.amg.gda.pl
2Department of Pharmaceutical and Medicinal Chemistry, Institute of Pharmacy, University of Greifswald, L.-John Str. 17, D-17487 Greifswald, Germany
3On leave from Medical University of Gdańsk

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Syntheses of novel N-amino-N′-(benzenesulphonyl)guanidines (4a–h, 5a–g) from N-(benzenesulphonyl)cyanamide potassium salt and hydrazine derivatives are described. Compounds 4b, 5a–c and 5e were evaluated by in vitro assays of growth inhibition against several human tumor cell lines. The highest in vitro cytotoxic activities were found for 3-phenylamino-1-(2-benzylthio-4-chloro-5-methylbenzenesulphonyl)guanidine (5b) (IC50 = 2.35–8.14 μM) and 3-phenylamino-1-(4-chloro-2-ethoxycarbonylmethyl-thio-5-methylbenzenesulphonyl)guanidine (5c) (IC50 = 2.74–10.6 μM), while other tested compounds (5a, 5e) showed the moderate cytotoxic activities. The molecular orbital calculation of the possible tautomeric forms of the benzenesulphonylguanidine derivatives were also presented.
Photophysics of Lumichrome and Its Analogs

by E. Sikorska¹, D.R. Worrall², J.L. Bourdelande³ and M. Sikorski⁴

¹Faculty of Commodity Science, Poznañ University of Economics, al. Niepodległości 10, 60-967 Poznañ, Poland; Fax: +48 61 8543993, Tel: +48 61 8569040, E–Mail: sikorska@novci1.ae.poznan.pl
²Department of Chemistry, Loughborough University, Loughborough, Leicestershire LE11 3TU, England
³Unitat de Quimica Organica, Universitat Autonoma de Barcelona, Barcelona 08193, Spain
⁴Faculty of Chemistry, A. Mickiewicz University, Grunwaldzka 6, 60-780 Poznañ, Poland

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The spectroscopic and photophysical properties of lumichrome and its 1- and 3-methyl and 1,3-dimethyl derivatives in acetonitrile and in methanol are presented. In common with the parent molecule, the photophysics of the lumichrome methyl derivatives are dominated by non-radiative transitions in both methanol and acetonitrile. However, fluorescence yields in methanol are higher than in acetonitrile as a result of a reduction in the efficiency of non-radiative deactivation channels. These observations are discussed in terms of the available solvent-solute interactions.
Neutron Spectroscopy, IR, Raman and Ab Initio Study of L-Proline

by A. Pawlukojć, J. Leciejewicz, I. Natkaniec and J. Nowicka-Scheibe

1 Joint Institute for Nuclear Research, 141980 Dubna, Russia
2 Institute of Nuclear Chemistry and Technology, 03 195 Warszawa, Poland
3 H. Niewodniczañski Institute of Nuclear Physics, Krakow, Poland
4 Institute of Fundamental Chemistry, Technical University, Szczecin, Poland

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Inelastic incoherent neutron scattering spectra (IINS) were obtained for normal and deuterated L-proline. Raman and infrared spectra were also recorded. Geometries were optimized for the zwitterion form using ab initio Hartree-Fock (HF) level with 6-31G*, 6-311G** and 6-311++G** basis sets. Force fields and normal modes were calculated and used as basis for an assignment of the spectral features. The theoretical frequencies of normal and d2 – L-proline were compared with IINS spectra.
The synthesis of derivative of poly (4-hydrazo-diphenylenedisulfide) by reaction of 1-chloro-4-nitrobenzene with sodium sulfide and disulfide in N-methyl-2-pyrrolidone leads to oligomeric products with average molecular weight of the homogeneous chains 1182 g/mol and 690 g/mol, respectively. The mechanisms of the reactive intermediates polycondensation reaction are described. The products were characterized by IR, 1H NMR, and EPR spectroscopy and by elemental analysis. The final amorphous oligomer products contain mostly diamagnetic species and about 1% of paramagnetic species. The latter produce strong isotropic EPR signal at \( g = 2.0025 \) from free radical with concentration of about \( 10^{18} \) radicals/gram. Pulsed EPR spectroscopy allowed identifying the radical by analysis of the electron spin echo envelope modulation spectrum. The radical is localized on the carbon atom of the C=O-group of the N-methyl-2-pyrrolidone moiety with broken internal C–N bond of the lactam ring.
Formation of Binuclear EDTA and Cu(II) Complexes in Aqueous Solutions

by O. Gylienė and J. Aikaitė

Department of Environmental Chemistry, Institute of Chemistry, Gottaauto 9, LT-2600 Vilnius, Lithuania, E-mail: gyliene@ktl.mii.lt

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Nickel/Alumina Catalyst for Carbon Oxides Methanation. Flash Calcination of the Catalyst Precursor

by R. Narowski, Z. Kowalczyk, J. Zieliński, A. Gołębiewski and K. Stolecki

1Warsaw University of Technology, Faculty of Chemistry, Noakowskiego 3, 00-664 Warsaw, Poland
2Institute of Physical Chemistry PAS, Kasprzaka 44/52, 01-224 Warsaw, Poland
3Fertilizers Research Institute, Al. Tysiąclecia P.P., 24-100 Pulawy, Poland

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Complexation Behaviour of 5(2′-Hydroxyphenyl)-3-phenylpyrazoline with Some Metallic Moieties

by U.N. Tripathi, K.V. Sharma, A. Chaturvedi and T.C. Sharma

1 Synthetic Inorganic and Organometallic Laboratory, School of Studies in Chemistry, Vikram University, Ujjain – 456 010, India
2 Department of Chemistry, Govt. PG. College, Ajmer, India

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Diffuse Reflectance Spectroscopy Applied to Solid-State 2-Methylsparteine Metal Complexes

by B. Jasiewicz¹, E. Sikorska², I.V. Khmelinskii³ and M. Sikorski¹

¹Faculty of Chemistry, A. Mickiewicz University, Grunwaldzka 6, 60-780 Poznañ, Poland
Tel: +48 61 8291309, Fax: +48 61 8658008, E-Mail: Sikorski@amu.edu.pl
²Faculty of Commodity Science, Poznañ University of Economics, al. Niepodległości 10, 60-967 Poznañ, Poland
³Universidade do Algarve, FCT, 8000–117 Faro, Portugal

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Phase Transitions in Guanidinium Bromoantimonate(V) 
[C(NH$_2$)$_3$]SbBr$_6$

by R. Jakubas, G. Bator and P. Ciapała

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

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