Faculty of Science

Department: Chemistry

Name: Raaat M. Issa

Title: Synthesis, characterization, thermal and antimicrobial studies of binuclear metal complexes of sulfa-guanidine Schiff bases

Authors: Raafat M. Issa, Saleh A. Azim, Abdalla M. Khedr & Doaa F. Draz

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Abstract:

A series of metal complexes of Schiff bases derived from condensation of sulfa-guanidine with 1-benzoylacetone (H_2L^1). 2-hydroxybenzopheonal (H_2L^2), dibenzoylmethane (H_2L^3) , 5-methylisatine (H_2L^4), and 1-methylisatine (H_2L^5) haave been synthesized. The complexes are characterized by elemental analysis, molar conductance, magnetic moment measurements, IR, UV-Vis, ^{1}H NMR spectra, as well as thermogravimetric analysis. The low molar conductance values indicate the complexes are nonelectrolytes. IR and 1H NMR spectra show that H_2L^1-H_2L^5 are coordinated to metal ions by two bidentate centers. Mn(II), Co(II), Ni(II), and Cu(II) complexes display paramagnetic behavior , whereas the Zn(II) complex was diamagnetic. All studies confirm the formation of an octahedral geometry for $[Cu_2L^1(AcO)_2(H_2O)_6.3H_2O$ (1). $[Mn_2L^4(AcO)_2(H_2O)_6].2H_2O$(6), $[Ni_2L^4(AcO)_2(H_2O)_2(H_2O)_6].2H_2O$ (8) a tetrahedral geometry for $[Cu_2L^2(AcO)_2(H_2O)_2]$ (2) $[Cu_2(L^4)_2]$, $pCo_2(L^4)_2.2H_2O$ (7) and $[ZnHL^4(AcO)(H_2O)$ (9) and a trigonal bipyramid geometry for $[Vi_2L^3(acO)_2(H_2O)_4]$ (3) and $[Cu_2HL^5$ $(AcO)_3(H_2O)_3$ (5). H2L4 was most effective on Gram negative, Gram positive bacteria, and fungi (diameters inhibition zone ranged between 10.5-27.5 mm) after 24 and 48 h. Complex 8 showed moderate antimicrobial activity. Its minimum inhibitory comcetntation (MIC) against Escherichia coli, Bacillus subtilis, Candida albicans and Aspargllus flavas was 20 mgL^{-1} . The compound proved to be of moderate toxicity and its LD50 ws 20 mgL^{-1}.

Keywords:

Sulfa-guanidine, Schiff bases, Metal complexes.

Faculty of Science

Department: Chemistry

Name:Raafat M. Issa

Title: Quantum chemical studies on the inhibition of corrosion of copper surface by substituted uracils

Authors: Raafat M. Issa, Mohamed K. Awad, & Faten M. Atlam

Published In:Applied surface science, 255,(2008)

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Abstract:

The inhibitive effect of some substituted uracils, dithiouracil (DTUr), thiouracil (TUr), uracil (Ur) and dihydrouracil (DHUr) against the corrosion of neutral copper surface is studied by means of density functional approach B3LYP/31G calculations. It is found that the DTUr inhibitor has the highest inhibition efficiency among the investigated inhibitors. The calculated quantum chemical parameters correlated to the inhibition efficiency are, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), the separation energy (E), the dipole moment (u) , the softness (o) , the fraction of the electrons transferred from the inhibitor to the metal surface (N) , the total negative charge (TNC), the molecular volume (v_i) and the total energy (TE). Also, the study of adsorption of the inhibitors on the neutral copper surface shows that the adsorption through the thiocarbonyl functional (C-S) group is more favored than the carbonyl group which agrees well with the experimental observations.

Faculty of Science

Department: Chemistry

Name: Raafat M. Issa

Title: 1H NMR, UR and UV/VIS spectroscopic studies of some Schiff bases derived from 2-aminobenzothiazole and 2-amnino-3-hydroxypyridine

Authors: Raafat M. Issa, Abdalla M. Khedr & Helen Rizk

Published In: Journal of the Chinese chemical society,55 (2008)

Impact Factor: 0.577

Abstract:

By condensing 2-aminobenzothiazole with 2-hydroxy-1-naphthaldehyde, 2-hydroxybenzaldehyde , 4-methoxybenzaldehyde, 4-hydroxybenzal-dehyde, benzaldehyde and 4-dimethylaminobenzaldehyde, and five Schiff bases Ia-Ie are prepped. Also , two Schiff bases IIa and IIb are prepared by condensation of 2-amino-3-hydroxypyridine with 2-hydroxy-1-napphthaldehyde and 2- hydroxybenzaldehyde. The ^{1}H , NMR, IR and UV/Vis spectra of these seven Schiff bases are investigated. The signals of the ^{1}H NMR spectra as well as the important bands in the IR spectra are considered and discussed in relation to molecular . The UV/Vis absorption bands in ethanol are assigned to the corresponding electronic transition and the electronic absorption spectra of Sciff bases Ib and IIb are studied in organic solvents of different polarities. The UV/Vis absorption spectra of 2-amino-3-hydroxypyridine Schiff bases IIa and IIb are investigated in buffer solutions of different pH values containing 5% (v/v) methanol, and the results are utilized for the determination of pKa and ΔG^* of the ionization of phenolic OH-groups . The fluorescence spectra of IIa and IIb are studied in organic solvents of different polrities.

The obtained spectral results are confirmed by some molecular calculations using the atom super position and electron delocalization molecular orbital theory for the Schiff base IIb.

Key words:

2-aminobenzothiazole ; 2-amino-3-hydroxypyridine; Benzaldehyde derivatives; Schiff bases; Spectral studies; Molecular orbital calculations.

Faculty of Science

Department: Chemistry

Name: R.M. Issa

Title: Supramolecular structures and stereochemical versatility of azoquinoline

AuthorsA.Z. El Sonbati , R.M. Issa & A.M.Abdel Gawad

Published In:Spectrochimica acta part A:(2007)

Impact Factor: 1.29

Abstract:

Rare earth complexes of 5-(phenylazo)-8- hydroxyqunoline (HL)of composition $[M(L)_2X\text{-}H_2O]$ [where M=La, Ce, Pr, Nd and $X=NO_3$ or NCS^-] have been prepared and characterized on the basis of their chemical analyses, ^1H NMR , magnetic measurements, conductance, and visible and IR spectral data. Composition, conductance and IR spectal data of the complexes show that the HL acts as a bidentate monobasic ligand. The visible spectra of Pr^{3+} and Nd^{3+} show characteristic f-f transitions, and the nephelauxetic effect 1- β of these transitions have been evaluated. These data indicate the weak involvement of the 4f orbitals in complex formation.

Faculty of Science

Department: Chemistry

Name: R.M. Issa

Title: Thermal studies of bis salicylidene adipic dihydrazone derivatives and their complexes with divalent ions of Mn, Co, Ni, Cu and Zn

Authors: R.M. Issa, S.A. Amer, I.A. Mansour and A.I. Abdel Monsef

Published In:J. of thermal analysis and calorimetry,90, (2007)

Impact Factor:1.425

Abstract:

The thermal stabilities of bis salicylidene adipic dihydrazone derivatives and their complexes with divalent Mn, Co, Ni, Cu and Zn were studied and discussed in terms of structure and type of metal ions. TG curves display mostly four steps of thermal decomposition. The first step is due to dehydration, then the elimination of the acetate anions followed by the decomposition of the ligand in two interacting steps. The activatin energies Ea were evaluated and discussed in accordance with the structure of the complexes which have been previously characterized by elemental analysis and IR specra. It was found that the activation energies of the com,plexes based on bis salicylidene adipic dihydrazone wre higher than those of the dihydroxy derivative.

Key words:

Activation energy, dihydrazons, metal complexes, thermal analysis