Faculty of Science

Department: ***Chemistry***

Name: ***Safaa El-Dun H. Etaiw***

Title: ***Effect of N-methylation on both ground and excited states properties of 1-(9-anthryl)-2-(2-benzothiazolyl) ethene***

Authors: ***Safaa El Din H. Etaiwl Mohamed K. Awad; Tarek A. Fayed & Morad M. El Hendawy.***

Published In:Journal of Molecular Structure 919(2009)

Impact Factor: 1.44

Abstract:

1-(9-anthryl)-2-(2-benzothiazolyl) ethane and its salt were synthesized to study the effect of quaternarization of the nitrogen atom of benzothiazole moiety on both ground and excited states properties such as spectral characteristicsx in different solvents and the geometrical and electronic structures. Dual emission was observed in both compounds which originated from the involvement of locally excited (LE) and twisted intermolecular charge transfer (TICT) or intermolecular exciplex formation in excited state. Semiempirical molecular orbital calculations (PM3 and ZINDO/Cl) were employed to calculate the geometrical and electronic structures of the investigated compounds in ground and excited states as well as their electronic transition. The direction of the intermolecular charge transfer was explored via the charge distribution on the individual molecular subunits in both ground and excited states, and from the orbital topologies of the HOMO and LUMO levels of the investigated compounds.

Faculty of Science

Department: Chemistry

Name: Safaa El Dine H. Etaiw

Title: Two spectrophotometric methods for the determination of clarithromycin in pharmaceutical formulations and human plasma based on charge transfer complexes.

Authors: Mohamed E. El-Zaria and Safaa El Din H. Etaiw

Published In: Canadian Journal of analytical sciences and spectroscopy, 52(6),(2007)

Impact Factor:0.5

Abstract:

Two novel, simple and sensitive spectrophotometric methods were applied successfully to the determination of clarithromycin (CLM) in pure, pharmaceutical dosage form, and humane plasma with good accuracy and precision. The methods were based on charge transfer complexes (CTCs) with both iodine (I_2) as o-acceptor and tetracyanoethylene (TCNE) as π-acceptor. The complexes were stable at least for two days after its formations. The orange and yellow CTC species have an absorption maxima at 363 and 420 nm for I_2 and TCNE, respectively, with a molar absorptivity between 2985 to 3497 and 6872 I mol^{-1} cm^{-1}. The stoichimetries of the CTCs were defined by Job's , molar ratio and straight line methods and were found to form 1:1 stable stoichiometric complexes. Also, the formation constants and thermodynamic parameters (Δ H , Δ S° and ΔG°) of the resulting CTCs were determined. The optimum reaction conditions and other analytical parameters were also investigated. The developed methods were found to be linear over concentration ranges of 35-135 and 15-95 ug ml^{-1} with a limit of detection 0.12 and 0.18 ug mL^{-1} for iodine and TCNE methods, respectively . The methods were shown to be applicable to the determination of CLM in human plasma.

Key words:

Charge transfer complexes, clarithromycin ; I_2 ; TCNE, UV-vis, drug analysis.

Faculty of Science

Department: Chemistry

Name: Safaa Rl-Din H. Etaiw

Title: Synthesis and crystal structures of three novel coordination polymers constructed from Ag(I) thioxyanate and nitrogen donor ligands

Authors: Safaa El Din H. Etaiw; Dina M. Abdel Aziz , Moustafa Sh. Ibrahim and Ahmed S. Badr El Din

Published In: Polyhedron, 28 (2009)

Impact Factor: 1.756

Abstract:

Three supramolecular coordination polymers (SCPs)(AgSCN)2L)(L-4,4'-bipyridine (bpy) (1), trans-1,2-bis(4-pyridyl) ethylene (tbpe) (2) and phenazine (phenz) (3) have been synthesized and structurally characterized by single-crystal X-ray diffraction. Synthesis was affected in H_2O/acetonitrile/NH_3 media at room temperature. The bpy, tbpe and phenz bipodal ligands adopt different conformations which would affect the skeleton of the (AgSCN)n building blocks that allow the interconnection of the (AgSCN)n fragments and propagation of the network structure in three dimensions. Supramolecular interacdtions such as hydrogen-Bonding, argentophilic interaction and π - π stacking play an important role in the assembly of these coordination polymers.

Faculty of Science

Department: Chemistry

Name: Safaa El-din H. Etaiw

Title: Self-assembly of supramolecular coordination polymers constructed from AgCn and bipodal spacers

Authors: Safaa El din H. Etaiw, Dina M. Ab El Aziz, and Ahmed S. Badr El-din

Published In:Elsevier 2009, Polyhedron, 2009, 28, 873-882

Impact Factor: 1.756

Abstract:

The synthesies and crystal structures of novel supramoleculr coordination polymers (SCPs) of AgCN with bipodal ligands; 4-4'-bipyridine (bpy), trans-1,2-bis(4-pyridyl0ethylene (tbpe) and 1,2-bis(4-pyridyl)ethane (bpy) are repoted. The syntheses were affected in H2O/acetonitrile)NH3 media at room temperature. SCP{(AgCN)2-bpy} (1) is monoclinic and crystallizes in the space group P2 1/c, a=9.0565 (4) A, b=16.0063(8)A, c=0.1361(4), B=110.51 and Z=4. SCP {(AgCn)3, (tbpe)2 .H2O } is triclinic and crystallizes in the space group P1, a=9.8427(4)A, b=14.0864(4), c=10.3596(6) A, =98.873, B=101.739, =95.506 and Z=2, SCP {(AgCN)4, bpe (3) is monoclinic and crystallizes in the space group P21/c, a=10.1982(5) A, b=9.1610(5) A, c=14.4862(6) A, B=130.00(18) and Z=2. The 3D-topolgies of 1-3 resulted from the ridging action of the bipodal ligands and the agrentophilic interactions as well as extensive H-bonding and -stacking.