Faculty of Science

Department:Chemistry

Name: M. Gaber

Title: Synthesis, spectral, thermal and theoretical studies of Cu(II) complexes with 3-[4-dimethylaminophenyl]-1-(2-pyridyl0prop-2-en-1-one (DMAPP).

Authors:M.Gaber, S.A. El Daly & Y.S.Y. El-Sayed

Published In:Journal of Molecular Strucutre, 922 (2009)

Impact Factor:1.44

Abstract:

Cu(II) complexes of 3-[4'-dimethylaminophenyl]-1-(2-pyridyl)prop-2-en-1-one (DMAPP) are prepared and characterized by elemental analysis as well as spectral studies (IR and UV-vis), ESR , magnetic susceptibilities and thermal studies. The effect of different alcoholic solvents as well as the temperature on the complex formation is studied. The effect of Cu(II) ion on the emission spectrum of the free chalcone is also assigned. The stoichiometry, stability constant, absorption maximum and molar absorptivity of the metal complexes as well as the effect of pH, temperature on complex formation are determined spectrophotometrically. Adherence to Beer's law and Ringbom optimum concentration ranges are determined. The thermal decomposition of the metal complexes is studied by TGA techniques. The kinetic parameters like activation energy, pre-exponential factor and entropy of activation are estimated. The structure of complex was energetically optimized through molecular mechanics applying MM+ force field coupled with molecular dynamics simulation.

Faculty of Science

Department: Chemistry

Name: M.Gaber

Title: Spectral properties and inclusion of 3-(4'-dimethylaminophenyl)-1-(2-furanyl) prop-2-en-1-one in organized media of micellar solutions, B-cyclodextrin and viscous medium.

Authors: M.Gaber , S.A.El-Daly & Y.S.El-Sayed

Published In:Journal colloids and surfaces B: biointerfaces 66(2008)

Impact Factor: 2.109

Abstract:

On the line of a previous work on the spectral properties of some of heteroaryl chalcone, the absorption and fluorescence emission spectral properties of 3-(4'-dimethylaminopheny)-1-(2-furanyl)prop-2-en-1-one (DMAFP), have been investigated in organized media of aqueous micellar and β-cyclodextrin (β-CD) solutions. While the absorption spectra are less sensitive to the nature of the added surfactant or β-CD, the characteristics of the intermolecular charge transfer (ICT) fluorescence are highly sensitive to the properties of the medium . The maximum is strongly blue-shifted with a great enhancement in the fluorescence quantum yield on adding micellar or β-CD. This indicates the solubilization of DMAFP in the micellar core and formation of an inclusion complex with B-CD. The critical micelle concentrations (CMC) as well as the polarity of the micellar core of SDS, CTAB and TX-100 have been determined . The CMC values are in good agreement with the reported values while the polarity is lower indicating that DMAFP molecules are incorporated in the micellar core not at the micellar interface. The inclusion constants of binding of DMAFP in micellar or B-CD have been also determined. The thermodynamic parameters of formation of DMAFP:CD inclusion complex have been calculated from the temperature dependence of the fluorescence spectra of the formed complex. The highly negative value of formation entropy ($S= 98.0$ J $mol^{-1}K^{-1}$) reflects the high restrictions imposed on the movement of both the host and included guest molecules which is consistent with the increase of the fluorescence yield and blue shift of the fluorescence maximum.

Faculty of Science

Department: Chemistry

Name: M. Gaber

Title: Spectral and thermal studies of new Co(II) and Ni(II) hexaaza and octaaza-macrocyclic complexes.

Authors: M.Gaber, A. Rehab & D.F. Badr-El-deen

Published In: J. Therm. Anal. Calor., 91, (2008)

Impact Factor:1.425

Abstract:

The macrocyclic comnplexes of Co(II) and Ni(II) having chloride or thiocyanate ions in the axial position have been synthesized and characterized. These complexes are synthesized by the template condensation of o-phenylenediamine or 2,3-butanedionedihydrazone with the appropriate aldehydes in NH_4OH solution in the presence of the metal ions, Co(II) and Ni(II) .The complexes were characterized by spectroscopic methods (IR, UV-Vis and ESR) and magnetic measurements as well as thermal analysis (TG and DTA). The results obtained are commensurate with the proposed formulae. Spectral studies indicate that these complexes have an octahedral structure. From conductivity measurements the complexes are non-electrolytes. The kinetic of the thermal decomposition of the complexes was studied and the thermodynamic parameters are reported.

Keywords:

Co(II), Ni(II) macrocyclic complexes, template condensation, thermal analysis.

Faculty of Science

Department: Chemistry

Name: M.Gaber,

Title: Spectroscopic studies of 4-(4,6-dimethylpyrimidin-2-ylazo) benzene -1,3-diol and its Cu(II) complexes.

Authors: M.Gaber, Tarek A Fayed, S.El Daly & Y.S.Y. El Sayed

Published In: Spectrochimica acta, (2007)

Impact Factor: 1.183

Abstract:

The electronic absorption spectra of 4-(4,6-dimethylpyrimidin-2-ylazo) benzene 1,3-diol have been studied in organic solvents of different polarities as well as in buffer solutions of varying pH. The observed UV-vis absorption bands are assigned to the corresponding electronic transitions. The effect of methanol ratio on the pK-value is discussed. Also, semiemperical molecular orbital calculations at the AMI level have been performed to investigate the molecular and electronic structures of the free ligand in the ground state. According to these calculations, an intramolecular hydrogen bond leads to increasing of the molecular stability. The important bands in the IR spectrum as well as the main signals in the ^{1}H NMR spectrum are also assigned. The interaction of Cu(II) on with the titled azo-dye in solution is studied spectrophotometrically and conductometrically. Optimization of the various experimental conditions is also described. Beer's law is obeyed in the range 0-11.43 ppm while that obtained applying Ringbom is 1.26 – 6.61 ppm. The use of the titled azo-dye as an indicator for determination of Cu(II) is considered. The solid Cu(II) complexes are synthesized and characterized by spectral, magnetic, conductance and thermal studies (TGA and DTA). The results indicate the formation of 1:1 and 1:2 (M:L) complexes. The kinetic parameters (n,E,A, ΔS, ΔH and ΔG) of the thermal decomposition stages were computed and discussed.

Key words:

Pyrimidine azo complexes, spectra, TGA , DTA , magnetic, conductance

Faculty of Science

Department: Chemistry

Name: M.Gaber

Title: Spectral properties and inclusion of hetero-chalcone analogue in organized media of micellar solutions and beta-cyclodextrin

Authors: M.Gaber, T.A. Fayed; S.A. ElDaly and Y.S. El Sayed

Published In: Photochemical and photobiological sciences, 7,257(2008)

Impact Factor: 0.564

Abstract:

The absorption and fluorescence emission spectral properties of 3-(4-dimethylaminophenyl)-1-(2-thienyl)prop-2-en-1-one, abbreviated as DMATP, have been investigated in organized media of aqueous micellar and β-cyclodextrin (CD) solutions. While the absorption spectra are less sensitive to the nature of the added surfactant or CD, the characteristics of the intramolecular charge transfer (ICT) fluorescence are highly sensitive to the properties of the medium. The ICT maximum is strongly blue-shifted with a great enhancement in the fluorescence quantum yield on adding micellar or CD solutions. The indicates the solubilization of DMATP in the micellar core and formation of an inclusion complex with β-CD. The critical micelle concentration (CMC) s well as the polarity of the micellar core of SDS , CTAB and TX-100 have been determined. The CMC values are in good agreement with the reported values while the polarity is lower indicating that DMATP molecules are incorporated in the micellar core not at the micellar interface. The inclusion constants of binding of DMATP in micellar or CD have been also determined. The thermodynamic parameters of formation of DMATP , CD inclusion complex have been calculated from the temperqature dependence of the fluorescence spectra of the formed complex. The negative enthalpy and free energy of formation indicate that the inclusion process is energetically favorable. The highly negative value of formation entropy ($\Delta S = -162.3$ mol^{-1} K^{-1}) reflects the high restrictions imposed on the movement of both and blue shift of the fluorescence maximum.

Faculty of Science

Department: Chemistry

Name: M. Gaber

Title: Photophysical properties, laser activity and photoreactivity of a heteroaryl chalcone. A model of solvatochromic fluorophore

Authors: M. Gaber, S.A. El Daly; T.A. Fayed & Y.S. El Sayed

Published In: Optics & Laser Technology (2008)

Impact Factor: 0.709

Abstract:

The absorption and fluorescence characteristics of 3-(4'-dimethylaminophenyl)-1-(2-thienyl)prop-2-ene-1 – one (DMATP) have been investigated in different solvents. DMATP dye exhibits a large red shift in both absorption and emission spectra as solvent polarity increases, indicating a large change in the dipole moment of molecules upon excitation due to an intramolecular charge transfer interaction. The fluorescence quantum yield depends strongly on the properties of the solvents, which was attributed to positive and negative solvatokinetic effects. A crystalline solid of DMATP gave an excimer like emission at 570 nm due to the excitation of molecular aggregates. This is expected from the idealized crystal structure of the dye that belongs to the B-type class of Steven's classification. A dye solution ca. 10^{-3} mol dm^{-3} in $CHCl_3$ gave a good laser emission in the range 480 -560 nm with emission maximum at 530 nm upon pumping by nitrogen laser (λ_{ex} = 337.1 nm). The excitation energy transfer from 7-dimethylamino-4-methyl coumarine (DMC) to DMATP has been also studied in ChCl3 and the values of energy transfer rate constant and critical transfer distance indicate a Forster-type mechanism. The photoreactivity and net photochemical quantum yield of DMATP in chlormethane solvents are also determined. We applied semiempirical Mo calculation using AMI and ZINO/S calculation to understand the geometric and electronic structure of DMATP molecule in both ground and excited states.

Key words:

Chalcone derivatives, Laser dye, energy transfer and solvatochromic

Faculty of Science

Department: Chemistry

Name: Mohamed Gaber

Title: Spectrophotometric, conductometric and thermal studies of Co(II), Ni(II) and Cu(II0 complexes with 2-(2-hydroxynaphthylazo)-4-hydroxy-6-methyl-1,3-pyrimidine

Authors: Mohamed Gaber, Ikhlas A. Mansour, and Yousif S.Y. El-Sayed

Published In: Spectrochimica acta part A:68 (2007)

Impact Factor: 1.29

Abstract:

The electronic absorption spectra of 2-(2-hydroxynaphthylazo)-4-hydroxy-6-methyl-1,3-pyrimidine in pure organic solvents of different polarities and in buffer solutions of varying pH are studied. The important bands in the IR and the main signals in the 1H NMR spectra are assigned. The observed uv-vis absorption bands are assigned to the corresponding electronic transitions. The molecular stoichiometry, stability constant, absorption maximum, molar absorptivity and Sandell's sensitivity of the complexes are calculated. Obeyence to Beer's law and Ringbom optimum concentration ranges are also determined. The ability of using the titled azodye as metalochromic indicator in complexometric titrations was also studied. The effect of Co(II), Ni(II) and Cu(II) ions on the fluorescence of the azodye is also considered. The solid Cu(II) complexes of the titled azodye have been prepared and characterized by elemental, IR, UV-vis spectra as well as by conductometric and magnetic measurements. The data suggest square plannar geometry for 1:1 and 1:2 (M:L) complexes. The thermal behaviour of the complexes has been studied. The kinetic parameters (n, E, A, ΔS and ΔG) of the thermal decomposition steps are computed using Coats-Redfer equations.

Key words:

Pyrimidine dyes; solvent effect, Buffer , Fluorescence, Compelxes.

Faculty of Science

Department: Chemistry

Name: M. Gaber

Title: Synthesis and characterization of Co(II) , Ni(II) and Cu(II) complexes involving hydroxyl antipyrine azodyes

Authors: M.Gaber; A.M. Hassanein & A.A. Lotfalla

Published In: J. of Molecular structure ,875(2008)

Impact Factor: 1.44

Abstract:

The complexes formed between some hydroxyl antipyrine azodyes and Co(II), Ni(II) and Cu(II) ions were studied spectrophotometrically in solution. The stoichiometry and stability constants of the metal chelates were determined . The spectrophotometric detrminattion of the titled metal ions and titration using EDTA were reported. The chelating behaviour of the azodyes was confirmed by preparing the solid chelates in which their structures are elucidated using molar conductance, elemental, thermogravimetric (TGA) analyses, IR, ESR and electronic spectra as well as the magetic measurements. Kinetic parameters are computed from the thermal decomposition data. The electrical properties for the metal complexes are measured from which the activation energies are calculated.

Key words:

Azoantipyrine, complexes, spectral and thermal studies.

Faculty of Science

Department: Chemistry

Name: M. Gaber

Title: Photophysical properties, excitation energy transfer and laser activity of 3-(4'-dimethylaminophenyl)-1-(2-pyridinyl) prop-2-en-1-one (DMAPP) – A new potential laser dye

Authors: S.A. El Daly, M. Gaber; S.S.Al Shihry & Y.S. El Sayed

Published In: J. of photochemical and photobiology A, 89 (2008)

Impact Factor: 2.286

Abstract:

The photophysical properties such as singlet absorption, molar absorptivity, fluorescence spectra, fluorescence quantum yield ($Ó f$) and transition dipole moment (μ_{12}) of 3(4'-dimethylaminophenyl)-1-(2-pyridinyl) prop-2-en-1-one (DMAPP) were measured in different media. DMAPP dye exhibits a large red shift in both absorption and emission spectra as solvent polarity increases, indicating a large change in dipole moment of molecule upon excitation. Also, the fluorescence quantum yield is solvent dependent. A crystalline solid of DMAPP gives excimer like emission at 585 nm. Dye solution ca $1x10^{-3}$ mole dm^{-3} in $CHCl_3$ gives a good laser emission in the range 440-600 nm with emission maximum at 550 nm upon pumping by nitrogen laser (λ_{ex} = 337.1 nm). The excitation energy transfer from 7-dimethylamino-4-methyl coumarine (DMC) to DMPP has also been studied in $CHCl_3$ and the value of energy transfer and critical transfer distance indicate a Forster-type mechanism . The photochemical quantum yields ($Ó_c$) of DMAPP in chloromethane solvents are also determined.

Key words:

3-(4'-dimethylaminophenyl)-1-(2-pyridinyl) prop-2-en-1-one ; laser dye, effect of solvents; fluorescence quantum yeidl and photoreactivity in chloromethane solvents.

Faculty of Science

Department: Chemistry

Name: M.Gaber

Title: Spectral and thermal studies of 4-(1H-pyrazolo {3,4-d} pyrimidin-4-ylazo)

Authors: M.Gaber, K.Y.El Baradie & Y.S. El Sayed

Published In:Spectrochimica Acta Part A: 69 (2008)

Impact Factor: 1.29

Abstract:

4-(1H-Pyrazolo{3,4-d} pyrimidin-4-benzene-1,3-diol was synthesized and characterized by various spectral and analytical techniques Semiempirical quantum calculations using the AM1 method have been performed in order to evaluate the geometry and electronic structure of the title azodye in the ground state. The complex formation between Co(II) and Ni(II) and Cu(II) ions and the title azodye ws studied conductometrically and spectrophotometrically. The spectrophotometric determination of the title metal ions and ttitration using EDTA are reported. Co(II) , Ni(II) and Cu(II) complexes of the title azodye have been synthesized and characterized by elemental analysis, conductivity, magntic susceptibility, IR, uv-vis and thermal analysis (TGA and DTA) . The spectral and magnetic data suggested the octahedral geometry for Co(II) and Ni(II) complexes while Cu(II) complexes have square planar geometry. The thermal studies confirmed the chemical formulations of the title complexes. The thermal degradation takes place in two or three steps depending on the type of the metal and the geometry of the complexes. The kinetics of the decomposition was examined by using Coats- Redferm relation. The activation energies and other activation parameters (ΔH, ΔS and ΔG) were computed and related to the bonding and stereochemistry of the complexes.

Key words:

Azody metal complexes; Co(II) Ni(II), Cu(II) , IR; ESR ; UV-Vis spectra; TGA; DTA