Solvatochromaticity and pH dependence of the electronic absorption spectra of some purines and pyrimidines and their metal complexes

Mamdouh S. Masoud [a], Medhat A. Shaker [b], Alaa E. Ali [b] , Gehan S. Elasal [b]

[a] Chemistry Department, Faculty of Science, Alexandria University, Egypt
[b] Chemistry Department, Faculty of Science, Damanhour University, Egypt

a b s t r a c t

The solvatochromic responses of uric acid (Ua), 6-amino-2-thiouracil (ATU) and a series of their complexes dissolved in ten solvents of different polarity have been measured. The solvent-dependent UV/Vis spectroscopic absorption maxima, _max, are assigned to the corresponding electronic transitions and analyzed using SPSS program, regression analysis and Kamlet and Taft methods. The observed solvatochromism is discussed using various solute–solvent interaction mechanisms. The electronic absorption spectra of ATU were investigated in aqueous buffer solutions of varying pH and utilized for the determination of dissociation constants. The ranges of pH, where individual ionic species are predominant have been determined.

Keywords:
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pH-effect

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Synthesis, computational, spectroscopic, thermal and antimicrobial activity studies on some metal–urate complexes

Mamdouh S. Masoud [a], Medhat A. Shaker [b], Alaa E. Ali [b] , Gehan S. Elasal [b]
[a] Chemistry Department, Faculty of Science, Alexandria University, Egypt
[b] Chemistry Department, Faculty of Science, Damanhour University, Egypt

a b s t r a c t

New sixteen uric acid metal complexes of different stoichiometry, stereo-chemistries and modes of interactions were synthesized using different metals Cr, Mn, Fe, Co, Ni, Cu, Cd, UO2, Na and K. The synthesized complexes were characterized by elemental analysis, spectral (IR, UV–Vis and ESR) methods, thermal analysis (TG, DTA and DSC) and magnetic susceptibility studies. Molecular modeling calculations were used to characterize the ligation sites of the free ligand. Furthermore, quantum chemical parameters of uric acid such as the energies of highest occupied molecular orbital (EHOMO), energies of lowest unoccupied molecular orbital (ELUMO), the separation energy (_E = ELUMO − EHOMO), the absolute electronegativity, _, the chemical potential, Pi, the absolute hardness, _ and the softness (_) were obtained for uric acid.

Eight different microbial categories were used to study the antimicrobial activity of the free ligand and ten of its complexes. The results indicate that the ligand and its metal complexes possess antimicrobial properties.

The stoichiometry of iron–uric acid complex was studied by using different spectrophotometric methods.

Keywords:
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