AIN SHAMS UNIVERSITY

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Physico-chemical studies on some transition metal chelates

A Thesis Submitted by

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For

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Under Supervision

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Title Sheet

Title : **physicochemical studies on some transition metal chelates**

Candidate : Hany Magdy Ahmed

Degree : Master of the Teacher's Preparation in Science (Inorganic Chemistry).

Department : Chemistry

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Name : Hany Magdy Ahmed

Title : physicochemical studies on some transitions metal chelates&molecular orbital calculations.

Submitted to : Chemistry Department, Faculty of Education, Ain Shams University

Abstract

$M(O\text{-}O)(N\text{-}N)_nX_n$, were prepared and characterized. The dissociation constants of HDMCHD as well as the formation constants of its complexes with some transition, lanthanide metal ions have been investigated potentiometrically in 50% (v/v) dioxane-water constant temperature .The thermodynamic parameters for HDMCHD chelate were evaluated and discussed. The data indicates monoprotic ligand and formation of complexes in molar ratio 1:1 and /or 1:2 (M:L). The solid metal complexes of the ligands with, Fe^{III}, Co^{II}, Ni^{II}, Cu^{II}, and Cd^{II} ions were isolated and characterized by elemental analysis, IR, electronic spectra as well as TGA, conductivity and magnetic susceptibility measurements. The data refer to the formation of monon or bi nuclear complexes and various geometries according to type of the metal ions as well as the ligand used. The optimized structures for the free ligands and their complexes have been determined using Hyper Chem 7.5 program at (*PM3*) level. The theoretical data gave good correlations with the experimental data.

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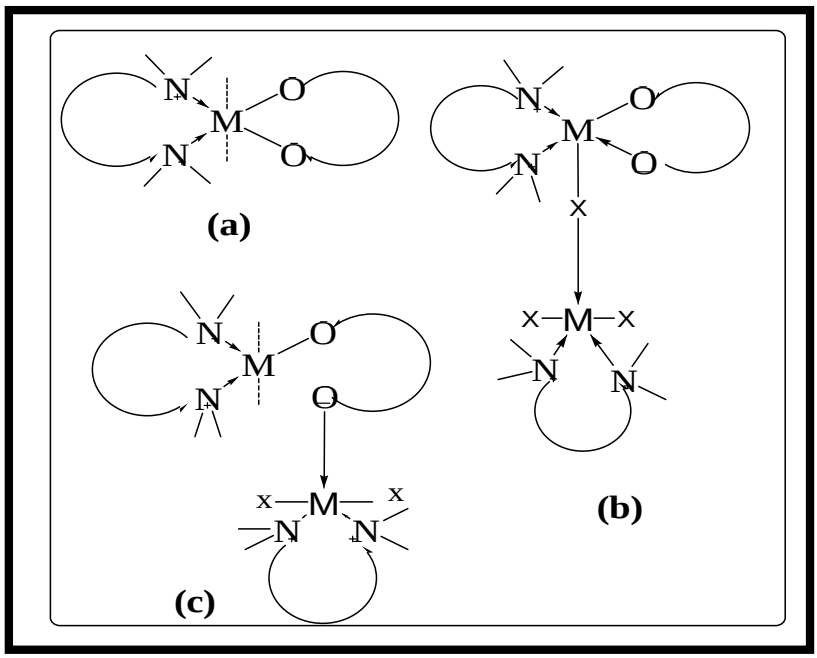
Aim of the Work

Complexes of the type M(O-O)(N-N) have been reported as antimicrobial activities, antibacterial, and antifungal activities However, the solvatochromic application of these complexes is very important . Owing to this paucity of information, we decided to investigate the reactivity and coordinating behavior and their solvatochromic application of these mixed ligand complexes.

The present study is planned to explore the dependence of coordination features and structure as well as solvatochromic behavior on the type of the metal cation and its counter anion as well as the experimental conditions of the current the copper(II) and Nickel(II)-complexes



Scheme I: The chelating modes of $M(O\text{-}O)(N\text{-}N)_nX_n$ complexes;

M= Cu(II) or Ni(II).

The present study comprises the following:

- Determination of the dissociation constant of 5,5-dimethyl cyclohexane1,3-dione ligand (HDMCHD) as well as stability constants of its complexes with some divalent transition and trivalent lanthanide metal ions using pH-metric technique in 50% (v/v) aqueous-dioxane-and isopropanol solutions at 25 ^{o}C and ionic strength 0.1M.

- i- Isolation and characterization of the solid complexes of the (O-O) and (N-N) mixed ligands with Ni^{II} and Cu^{II} metal ions. The characterization based on the microanalytical, spectral, magnetic, molar conductance and thermal studies.

  ii- Investigation of the solvatochromic properties of the isolated complexes in various organic solvents .

- Molecular orbital calculations of the present ligands and their copper(II) complexes using Hyper Chem 7.5 program at parametric method (*PM3) level*; and correlate the calculated structural parameters with the experimental data

- Antimicrobial screening of the present complexes toward some Gram–positive and Gram–negative bacteria; yeast and fungus**.**

Approval Sheet

Title : physicochemical studies on some transitions metal chelates

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Degree : master degree. of the Teacher's Preparation in Science (Inorganic Chemistry)

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Post Graduate Studies

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List of puplications

A. Taha, A.A.Taha and H.M.Ahmed 15-military college conference 2013.

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List of abbreviations

H_2pheth	Phethalic acid
H_2Saly	Salicylic acid
H_2Suc	Succinic acid
H_2Ox	Oxalic acid
Hgly	Glycine
H aspi	Aspirin(acetylsalicylic acid)
HOHAP	O-hydroxy acetophenone
Hmesalt	Methylsalicylate
HDMCHD	5,5dimethylecyclohexane,1,3dion
HEAA	Ethyl acetoacetate
en	ethane-1,2-diamine
Me_3en	N,N,N'-trimethylethylenediamine
Me_4en	N,N,N`,N`-tetramethylethylenediamine
Me_5dien	N,N,N',N'N"-pentamethyldiethylenetriamine
ΔHf	Heat of formation
HOMO	High Occupied Molecular Orbital
LUMO	lowest Unoccupied Molecular Orbital
BZ	Benzene
dmp	2,9-dimethyl-1,10-phenanthroline
pydcH_2	pyridine-2,6-dicarboxylic acid
tpmc	N,N,^{0}N",N"^{0}-tetrakis-(2-pyridylmethyl)-1,4,8,11-tetra azacyclotetra decane
acac	acetylacetonate
TAE	tetraacetylethane
SMLR	stepwise multiple linear regression
H_2Mal	malonic acid
DEtEMal	diethylethoxyethylenemalonate
1,3-pn	1,3-propylenediamine
Et_3en	N,N,N′-triethylethylenediamine
Me_4pn	N,N,N′,N′-tetra-methylpropylenediamine
medach	N-methyl-1,4-diazacycloheptane
bzac	benzoylacetonate
bipy	2,2'-bipyridine
phen	1,10-phenanthroline
H_2DACR	4,6-diacetyl-resorcinol
HOHBZ	o-hydroxy benzaldhyde

List of Schemes

List of Structures