

STUDY OF THE REACTIONS OF SOME METAL CARBONYLS WITH SOME QUINOXALINE DERIVATIVES

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Presented By

Khalifa Abdoalsalam Alfallous

M.Sc. in Chemistry (2004)

Under Supervisions of

Prof. Dr. Mohammed Fathi El-Shahat

Professor of Inorganic and Analytical Chemistry
Faculty of Science, Ain Shams University

Dr. Attia S. Attia

Assistant Professor of Inorganic Chemistry
Faculty of Science, Ain Shams University

Dr. Mostafa Yassen Nassar

Lecturer of Inorganic Chemistry
Faculty of Science, Banha University

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بسم الله الرحمن الرحيم

" وَيَسْأَلُونَكَ عَنِ الرُّوحِ قُلِ الرُّوحُ
مِنْ أَمْرِ رَبِّي وَمَا أُوتِيتُمْ مِنَ الْعِلْمِ
إِلَّا قَلِيلًا "

صدق الله العظيم

سورة الإسراء
آية (85)



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of the quinoxaline-2,3-dione ligand and 2,2'-bipyridine as a co-ligand: Syntheses, spectral characterizations, magnetic properties, antimicrobial inhibitory activities and interpretation of the electronic absorption spectra using the ZINDO/S-CI semi-empirical method

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LIST OF ABBREVIATION

Abbrev.	Full term
bpy	2,2' - bipyridine
¹HNMR	Proton Nuclear Magnetic Resonance
DCQX	6,7-dichloroquinoxaline-2,3-dione
DMF	Dimethyl formamide
DMQX	6,7-dimethylquinoxaline-2,3-dione
DMSO	Dimethyl sulphoxide
EtOH	Ethyl alcohol
IR	Infra-red
PM3	Semiempirical methods
QX	Quinoxaline
THF	Tertahydrofuran
UV-Vis	Ultraviolet-Visible
μ_{effct}	Effective Magnetic Moment



SUMMARY

SUMMARY

Complexes of chromium, molybdenum and ruthenium with derivatives of quinoxaline ligand, namely 6,7-dichloroquinoxaline-2,3-dione (DCQX) and 6,7-dimethylquinoxaline-2,3-dione (DMQX) have been synthesized and characterized.

Two novel complexes (bisdipyridine-quinoxaline derivatives-tricarbonyl dimolybdenum (0) of the general formula $\text{Mo}_2(\text{bpy})_2(\text{QX})(\text{CO})_3$, (where $\text{QX} = \text{DCQX}$ or DMQX) and $\text{bpy} = 2,2'$ -bipyridine), was synthesized in two steps starting with the reaction of $\text{Mo}(\text{CO})_6$ with bpy then followed by the addition of QX ligand. Initial characterization based on the elemental and mass analyses has suggested three possible structures. In the three suggested structures the QX ligand bonded to two $\text{Mo}(0)$ metal centers; to one Mo metal through its $\text{C}=\text{O}$ functional groups and the other through the aromatic ring forming η^6 -arene type. In one of the suggested structures the QX ligand is bonded to $(\text{bpy})_2\text{Mo}$ and $\text{Mo}(\text{CO})_3$ moieties, whereas in the other structures the QX ligand is bonded to $\text{Mo}(\text{bpy})(\text{CO})$ and *cis*-($\text{bpy})(\text{CO})_2\text{Mo}$ or *trans*-($\text{bpy})(\text{CO})_2\text{Mo}$) moieties. The IR studies were useful in assigning the coordination modes of the ligands especially in the carbonyl region of the spectrum. ^1H NMR studies in DMSO-d_6 displayed typical patterns corresponding to *cis*-($\text{bpy})_2\text{M}$ moiety. The electronic absorption spectrum of the complexes revealed two bands assignable to $\text{Mo}(\text{d}_\pi) \rightarrow \text{arene}(\pi^*)$ and $\text{Mo}(\text{d}_\pi) \rightarrow \text{bpy}(\pi^*)$

MLCT transitions. The thermogravimetric analysis gave more insight into the composition and the thermal stability of the complexes. The structural and vibrational behaviors of the $\text{Mo}_2(\text{bpy})_2(\text{DCQX})(\text{CO})_3$ complex have been elucidated using semiempirical parameterized PM3 method. The biological activity studies revealed higher antimicrobial inhibition of $\text{Mo}_2(\text{bpy})_2(\text{DCQX})(\text{CO})_3$ complex compared with the free DCQX ligand. Whereas, the $\text{Mo}_2(\text{bpy})_2(\text{DMQX})(\text{CO})_3$ complex showed only higher antifungal inhibitory activities compared with the free DMQX ligand.

With chromium hexacarbonyl $[\text{Cr}(\text{CO})_6]$, two new diethoxo-bridged dinuclear Cr(III) complexes $[\text{Cr}(\text{QX})(\text{bpy})\text{EtO}]_2$ have been synthesized and characterized. The complexes were initially characterized on the basis of their elemental and mass analyses. The infrared studies were useful in assigning the coordination mode of the quinoxaline-2,3-dione ligand to the chromium metal. In addition, the presence of μ -ethoxo bridges was inferred from the characteristic vibrational bands in the IR spectra of both complexes. The structural and vibrational behaviors of both complexes have been elucidated using parameterized PM3 semiempirical method. The magnetic susceptibility measured at 298 K has indicated exchange interactions between the two Cr(III) centers. The observed effective magnetic moments have been correlated to the calculated Cr...Cr distances and Cr–O–Cr angles of the $\text{Cr}(\text{OEt})_2\text{Cr}$ cores in both complexes. The ESR spectra have been recorded on powder samples at 298 K. The dominant quintet state