Novel Metal Complexes Derived From N_2S_2 Donor Sets; Synthesis, Structural Characterisation and Biological Activities

Baidaa K. Al-Rubaye [a], Riyadh M. Ahmed [a], Enaam I. Yousif [a], Mohamad J. Al-Jeboori [a*] and Herman Potgieter [b]

[a]Department of Chemistry, College of Education for Pure Science (Ibn Al-Haitham), University of Baghdad, Baghdad, Iraq
[b]Division of Chemistry and Environmental Science, Manchester Metropolitan University, Manchester, M1 5GD, UK

E-mail: ***mohamadaljeboori@yahoo.com***

University of Baghdad

Introduction

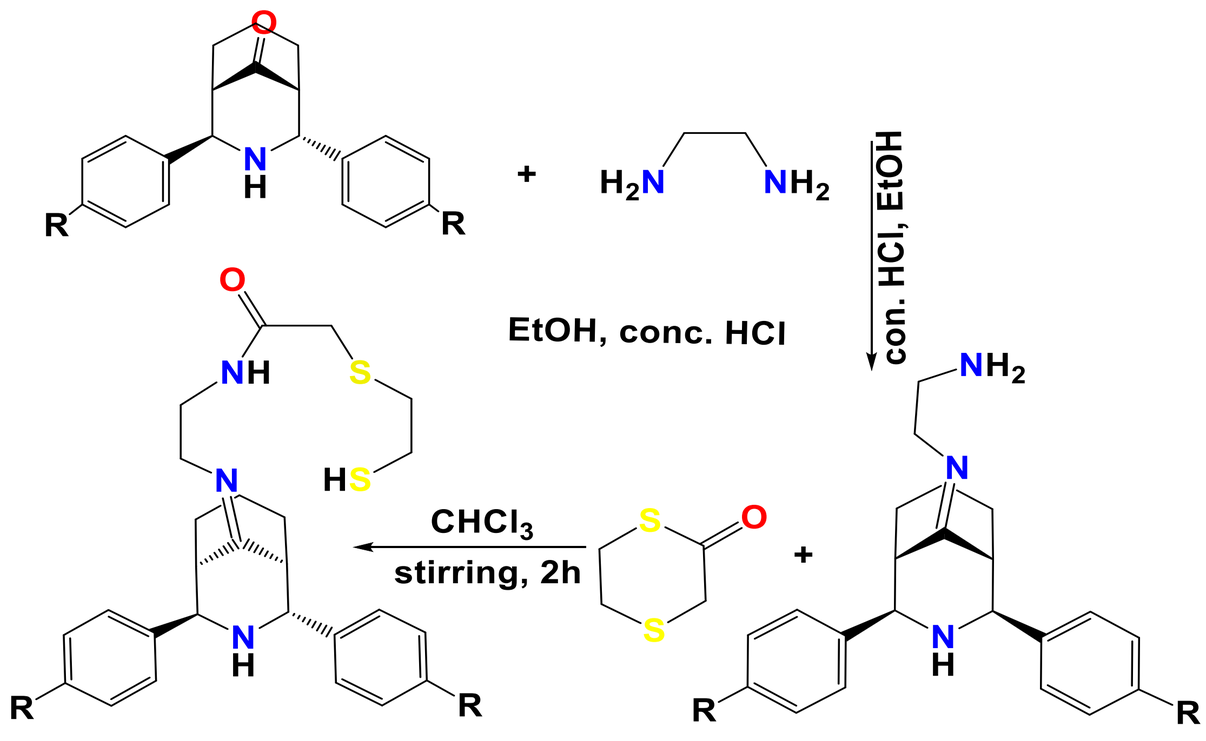
Compounds that contain nitrogen and sulfur in their structures are a class of organic species that attracted a range of chemist researchers (organic, inorganic and bioinorganic chemists) [1]. The impact of these species on chemistry stimulated researches to investigate and implement a range of synthetic protocols to increase yields and stability of these materials. These species have shown a range of potential applications, including their role as useful chelating agents for transition and representative elements [2], in medicine [3], as a mimic for bioactive molecules, in catalysis, analytical chemistry, coordination chemistry [4], environmental, materials and supramolecular chemistry [5].

Aim

The aim of this work is to produce polydentate ligands with N_2S_2 chelate system and their complexes and studying their biological activity. The ligands incorporated in their structure amid, imine, thiolate and thioether moieties.

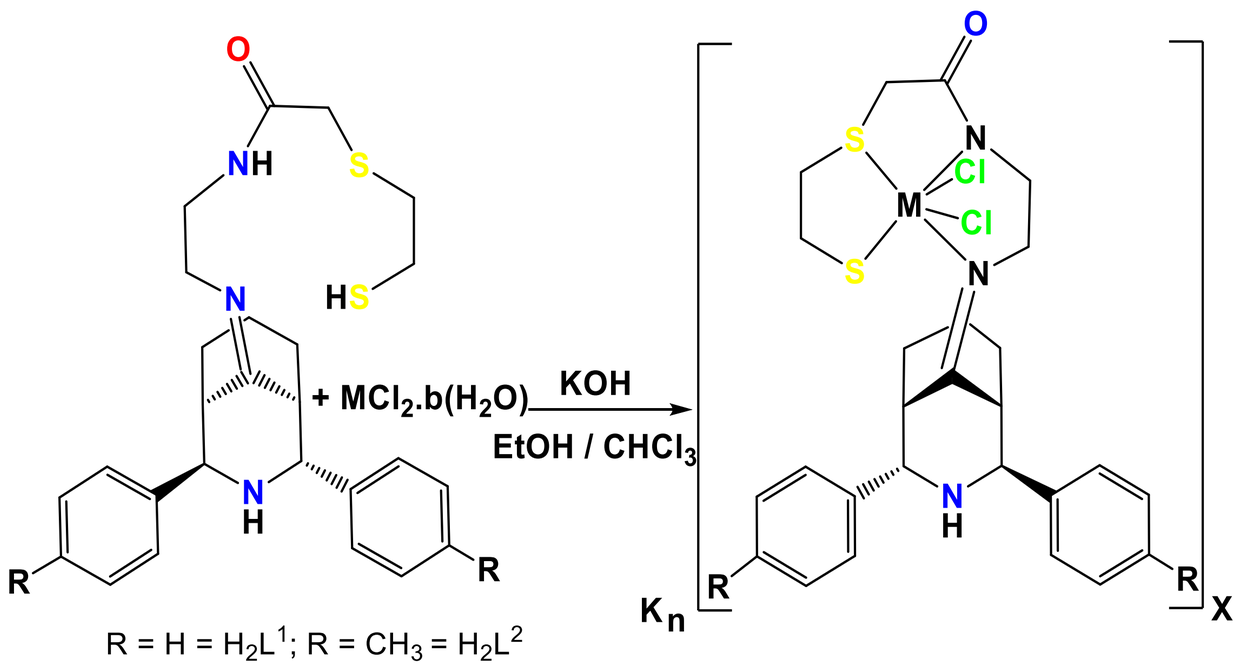
Experimental Procedure

The ligands were prepared from the reaction of 1,4-dithian-2-one with the appropriate azabicyclo[3.3.1] nonan-9-ylidene)amino)ethan-1-amine precursors, Scheme 1. Metal complexes were prepared in ethanolic solution. Metals chloride 1eq was added dropwise to the solution of 1eq of the appropriate ligand in EtOH, and then heated at reflux under N2 for 3h, Scheme 2. A solid that formed was filtered, washed by ethanol and diethylether, and dried under reduced pressure.



R = H = H_2L^1; R = CH_3 = H_2L^2

Scheme (1): Synthetic route for ligands of (H_2L^1 & H_2L^2).



R = H = H_2L^1; R = CH_3 = H_2L^2
M = Mn(II), Co(II), Ni(II); n = 2; X = 0
M = Cu(II), Zn(II), Cd(II); n = 0; Cl = 0; X = 0
Except; M = Cu(II); R = CH_3 = H_2L^2; Cl = 0; n = 0; X = Cl
b = Number of water molecules

Scheme (2): Synthesis of metal complexes.

Results & Discussion

Compounds were fully characterised using a range of analytical and spectroscopic techniques. Theoretical approach was used to confirm the coordination mode and the preferred geometry arrangement around metal centre. The optimization studies indicated that complexes of H_2L^1 and H_2L^2 preferred the six coordinate geometry (for Mn(II), Co(II), Ni(II)) of these ligands. While, the Cu(II), Zn(II) and Cd(II) complexes of H_2L^1 and H_2L^2 preferred the four coordinate geometry, the more stable arrangement. Biological assay indicated ligands and their complexes displayed different activity effect on bacterial strains (Gram positive (G+) and Gram negative (G-)) and fungi species, Figure (3: A and B).

Conclusions

The synthesis and coordination chemistry of some complexes obtained from reaction of multidentate N_2S_2 heterocyclic ligands H_2L^1 and H_2L^2 with a range of metal ions are explored. The experimental and theoretical studies indicated the formation of six and four coordinate metal complexes. Biological activity were also investigated.

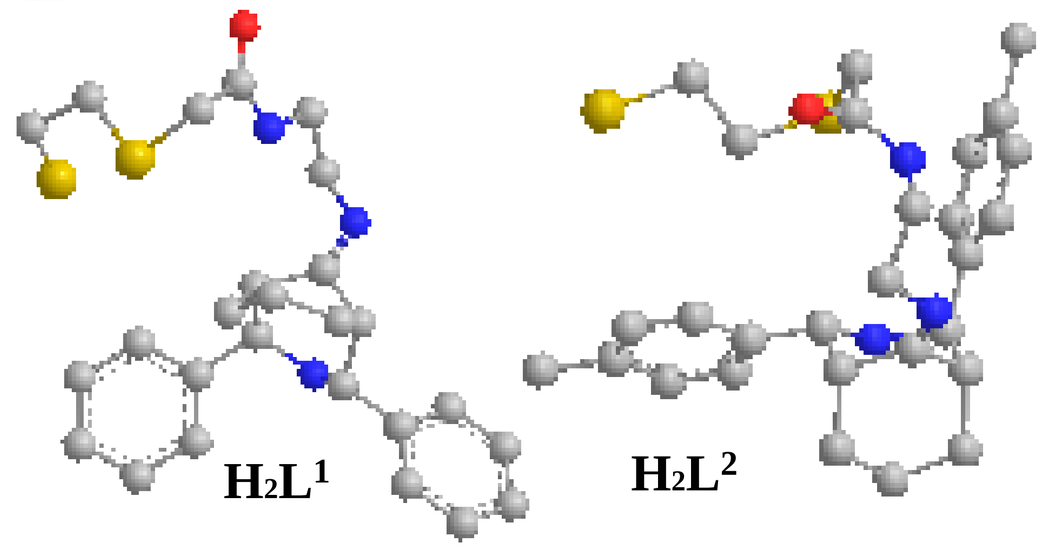


Figure (1): Optimized molecular structure of H_2L^1 & H_2L^2

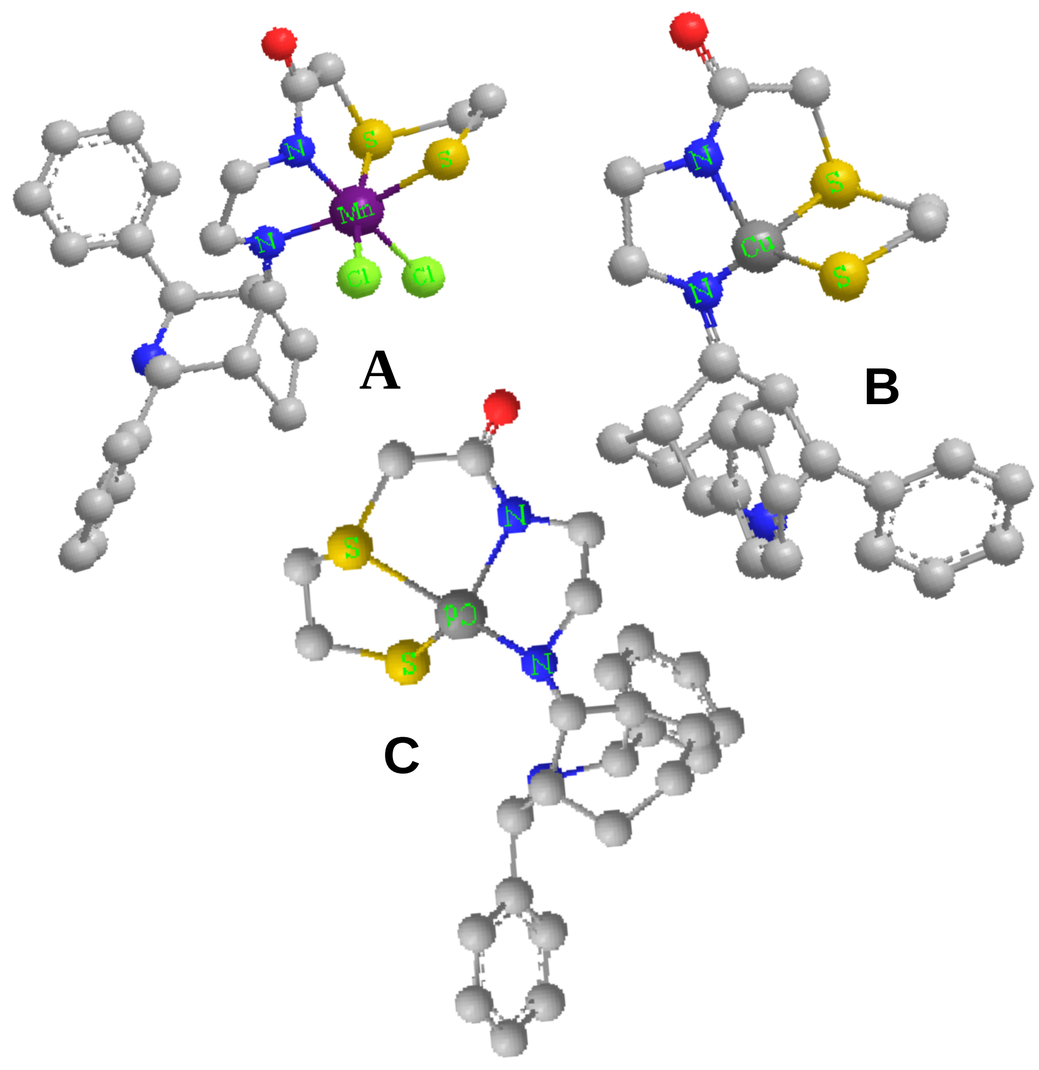


Figure (2): Optimized molecular structure of octahedral geometry $K_2[Mn(L^1)Cl_2]$ (A), square geometry $[Cu(L^1)]$ (B) and tetrahedral geometry $[Cd(L^1)]$ (C).

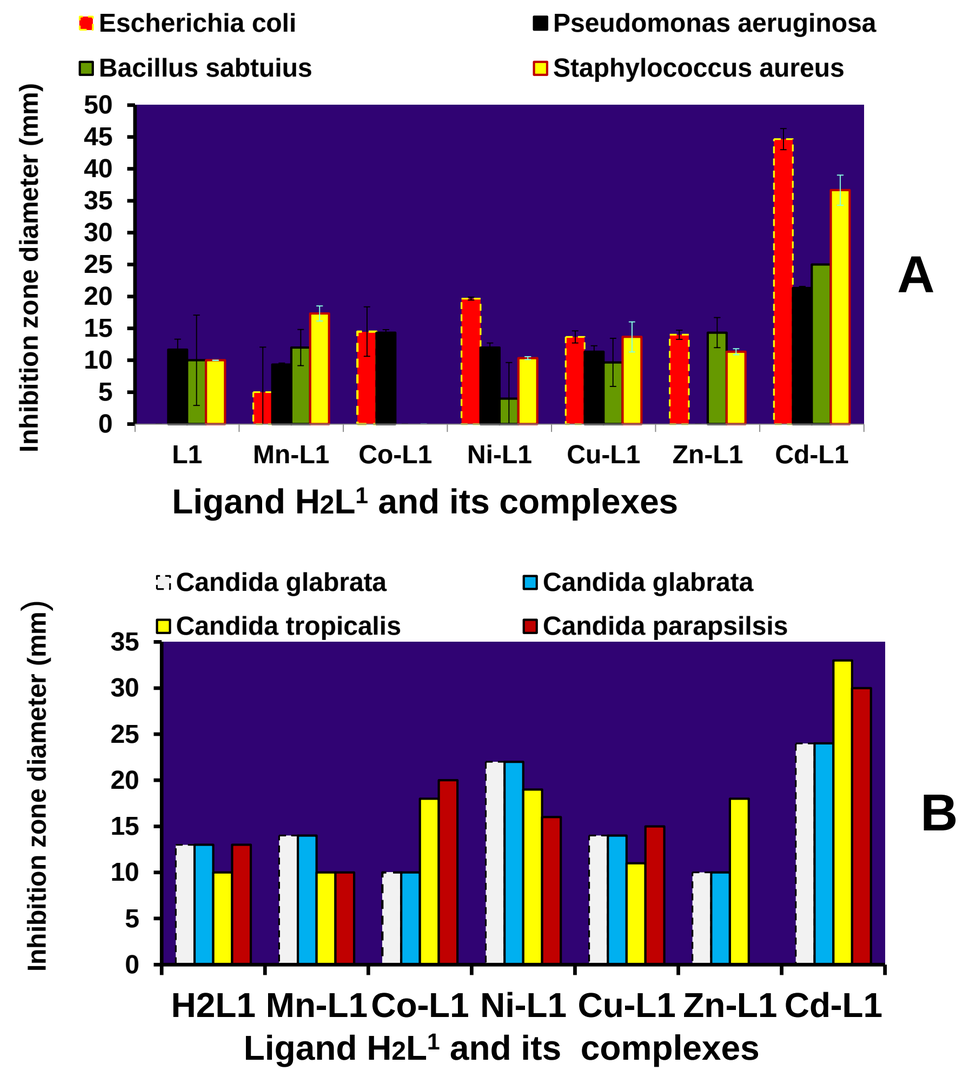


Figure (3): Evolution of inhibition diameter (mm) of (H_2L^1) and its complexes against the growth of tested bacterial strains (A) and fungi species (B).

References

[1] A. K. Asatkar, M. Tripathi, S. Panda, R. Pande and S. S. Zade, *Spectro Chimica Acta Part A: Molecular and Biomolecular Spectroscopy,* **171**, 18-24, (2017).

[2] J. W. Thaddeus, H. W. Edward, R. W. Gary, and J. Carolyn, *A. Chem. Rev.,* **110**, 2858–2902, (2010).

[3] U. Abram, and R. Alberto, *J. Braz. Chem. Soc.,* **17**, 8, 1486-1500, (2006).

[4] A. Yokoi, N., Yoshinari and T. Konno, *J. Incl. Phenom. Macrocycl Chem.*, **82**, 123-133, (2015).

[5] A. T. Bilgin, B. Ertem, Y. Gok, *Dyes and Pigments,* **80**, 187-193, (2009).

Acknowledgment

The authors would like to thank the Iraqi Ministry for Higher Education and University of Baghdad for the providing of the funding for the project.