



Detection of Divalent Heavy Metal in Wastewater Promoted by the Chelating Ability of Dimethylglyoxime Ligand Using Computational Method: DFT Analysis

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1 INTRODUCTION

More than 2/3 of our planets is covered by water. Globally, over 80% of all wastewater from our homes, industries flows back to nature without being treated or reused-polluting the environment. Heavy metal pollution has become one of the most serious environmental problems today [1] because they are toxic substances with carcinogenic nature thus should not to be discharged directly into the environment [2]. For ages, different methods have been used, each method has its own heavy metal removal efficiencies and the specific parameters that affect the removing and also inherent limitations such as the generation of a large amount of sludge, low efficiency, expensive electricity. Previously, dimethylglyoxime ligand has been used to detect Ni and the complexation of metals and thus removal [3]. This is because of the excellent coordination ability of transition metal with oxime and ability to form a stable



Scheme1.Fwater-quality-in-cameroonproject.org

CONNECTION TO SDGs



SDG 3 – Good Health and well being
SDG 6 – Clean water and sanitation



How to render a reliable contribution to the understanding and knowledge of the intrinsic elements of the electronic activity of glyoxime complex in the removal of heavy metal

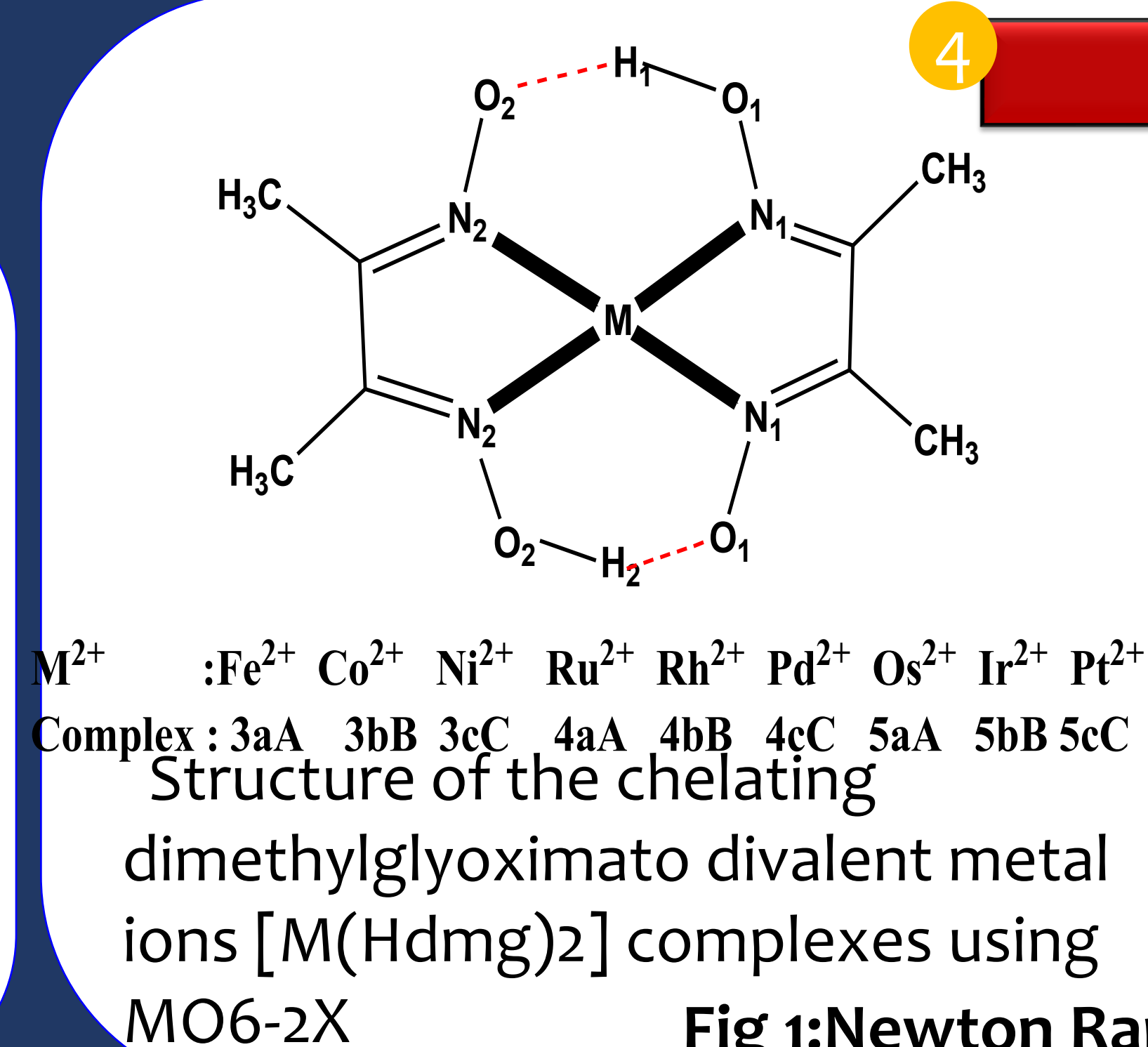
2 OBJECTIVES

- ❑ To optimise the geometry and energy minimisation of a selective range of complexes
- ❑ To assess the thermodynamic parameters
- ❑ To study the electronic and spectral properties
- ❑ To propose a suitable and effective ligand model for the detection and removal of metal ions from wastewater

3 MATERIALS

- Hardware infrastructures
- Desktop system: PC (Dell Pentium (R) dual Core with 2GB RAM.
- LAPTOP SYSTEM: PC (Dell Pentium (R) dual Core with 3GB RAM
- SOFTWARE INFRASTRUCTURES
- Gaussian 16, Revision B.01 program package. [3]
- Gauss View package/multiwfn software package. /ChemOffice package /Origin software package.

4 METHODOLOGY



GEOMETRY OPTIMIZATION

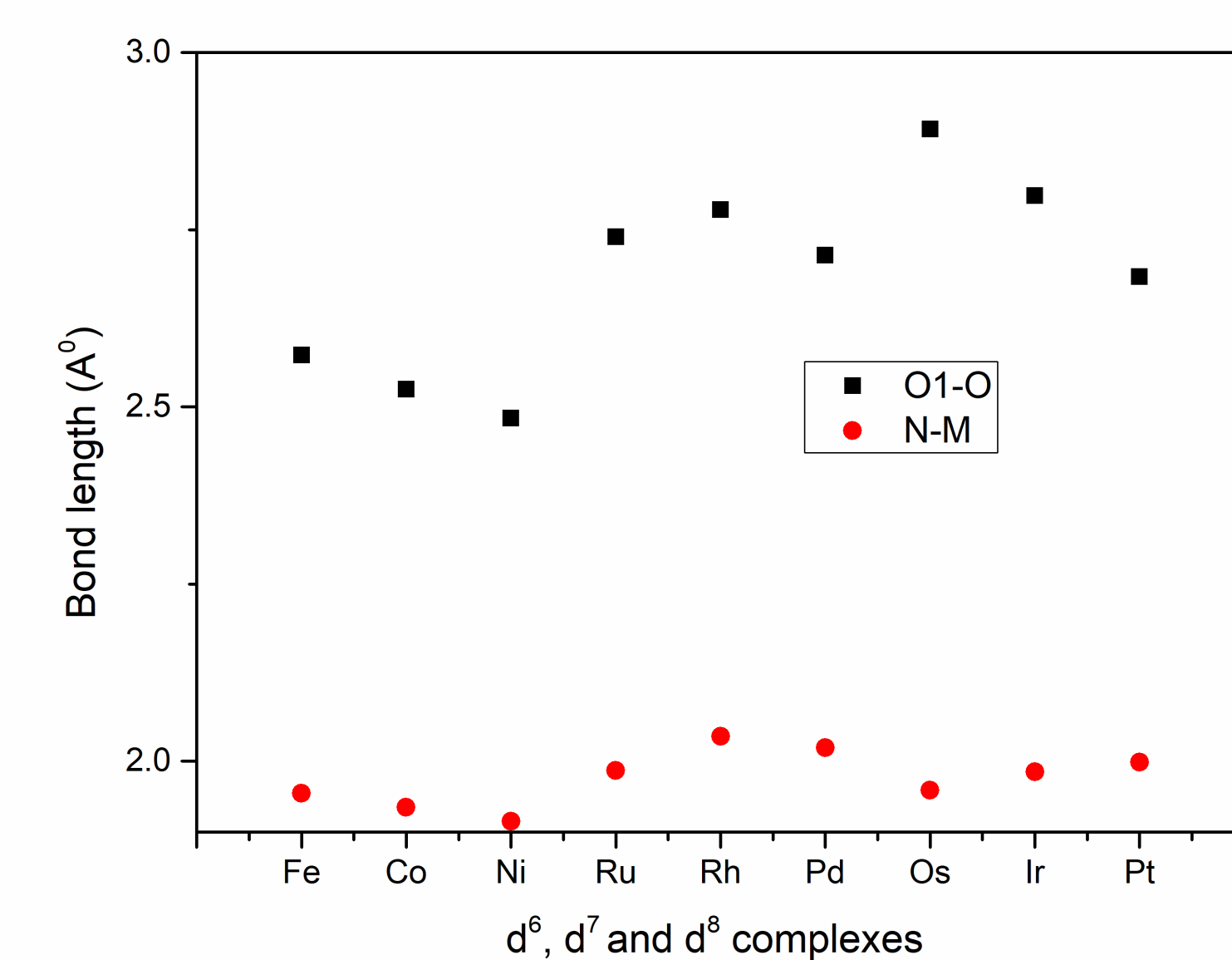
Fig 1: Newton Raphson Optimization

SPECTRAL PROPERTIES ANALYSIS

MOLECULAR STRUCTURAL ANALYSIS



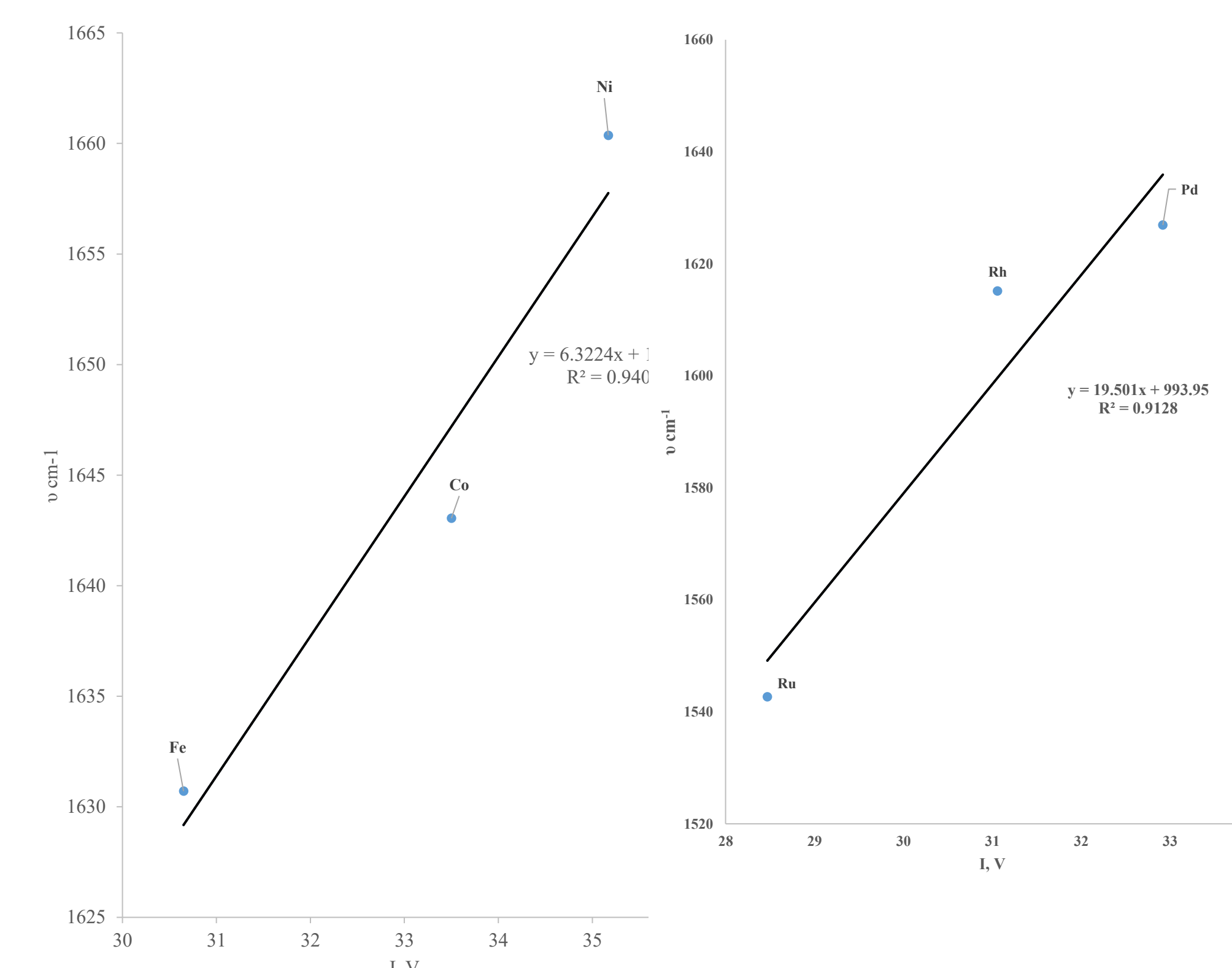
5 RESULTS



Tab1: IR analysis of selected computed bending and stretching vibrational IR frequencies

Complex	O1-O	N-M	O1-O	N-M	O1-O	N-M
Fe	1594.76	1594.76	1594.76	1594.76	1594.76	1594.76
Co	1677.56	1677.56	1677.56	1677.56	1677.56	1677.56
Ni	1693.27	1693.27	1693.27	1693.27	1693.27	1693.27
Ru	1690.14	1690.14	1690.14	1690.14	1690.14	1690.14
Rh	1690.14	1690.14	1690.14	1690.14	1690.14	1690.14
Pd	1690.14	1690.14	1690.14	1690.14	1690.14	1690.14
Os	1690.14	1690.14	1690.14	1690.14	1690.14	1690.14
Ir	1690.14	1690.14	1690.14	1690.14	1690.14	1690.14
Pt	1690.14	1690.14	1690.14	1690.14	1690.14	1690.14

Fig1:
increasing bond length
MO6-2X/Gen selected bond distances of optimized structures of complexes
Ni < Co < Fe < Os < Ir ≈ Ru < Pd < Pt < Rh



The strength of hydrogen bridges
Co>Ni>Fe>Pt>Pd>Rh>Ru>Ir>Os

6 CONCLUSION

- Globally, according to NBO the hybridizations of the metal cation within complexes for M-N bonds are ~dsp² interacting suggesting a square planar environment of complexes,
- The molecular geometries were computed using Mo6-2X functionals in DFT method at the 6-311+G(d,p)/Lan1D2Z basis set. Geometrical results obtained indicate that O...O separation distance (upper than 2.5Å) increase along the Co>Ni>Fe>Pt>Pd>Rh>Ru>Ir>Os
- proved the asymmetric character of the two formed O-H...O intramolecular H-bonds within the complexes. The examination of M-N bonding interactions reveal that the σ-bonding orbitals are slightly polarized toward the nitrogen atom
- The electronic calculated results based on bonding properties analysis according to QAIM and NBO calculations reveal that, the nature of the metal as well as the presence of asymmetric intramolecular H-bond which connect the two Hdmg ligands in the completely planar molecules determine the chemical and thermodynamic stability. The energy of the hydrogen bond of the complexes is responsible for their stability.
- The CN frequencies, in this column, the transfer of d-electrons in the direction Me → N=C increases with atomic number
- -π* character with a marked metal-to-ligand charge transfer (MLCT) contribution

7 REFERENCES

1. Fu et al., 2011
2. Hunsom et al., 2005; Adhoum et al., 2004
3. Yegani et al., Acta Biologica Turcica 30(1) 22-26, 2018
4. Gaussian 16: Revision A.2, Gaussian, Inc.; wallingford CT 2009.

8 ACKNOWLEDGEMENTS

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