

A concise description of supplementary

materials of paper entitled:

Transition Metal Complexes of Mixed Bioligands: Synthesis, Characterization, DFT Modeling and Applications

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The supplementary materials contain six figures and two tables to more clarify the structures and trends of the new preparing metal ternary complexes.

Figure Captions:

Figure 1S. Infrared spectra of ligands (glutamic, arginine) and [Zn.Glu.Arg.(H₂O)₂].H₂O.

Fig 2S. mass spectrum of Zn(II) complex

Figure 3S. The EPR spectrum of the Cu(II)-complex

Figure 4S. EPR Mulliken spin populations and Hyperfine (HF) coupling constants between Co(II)- and Cu(II)-ions bearing the unpaired electron and the surrounding O and N atoms of the chelates. HFC Values in MHz (1 MHz=0.00033356 cm⁻¹).

Figure 5S. Some Photos of some microbial activity for the prepared complexes.

Figure 6S. The inhibition efficiency of aluminum specimens in aqueous solution of 1M HCl with different concentrations of mixed ligands (glu.and arg.)and their ternary metal complexes at 303K for 7 h.

• **Table Headings:**

Table 1S. MIP (molecular ion peak) values from mass spectra of the prepared complexes.

Table 2S. Cytotoxicity evaluation of the ligands and their complexes.

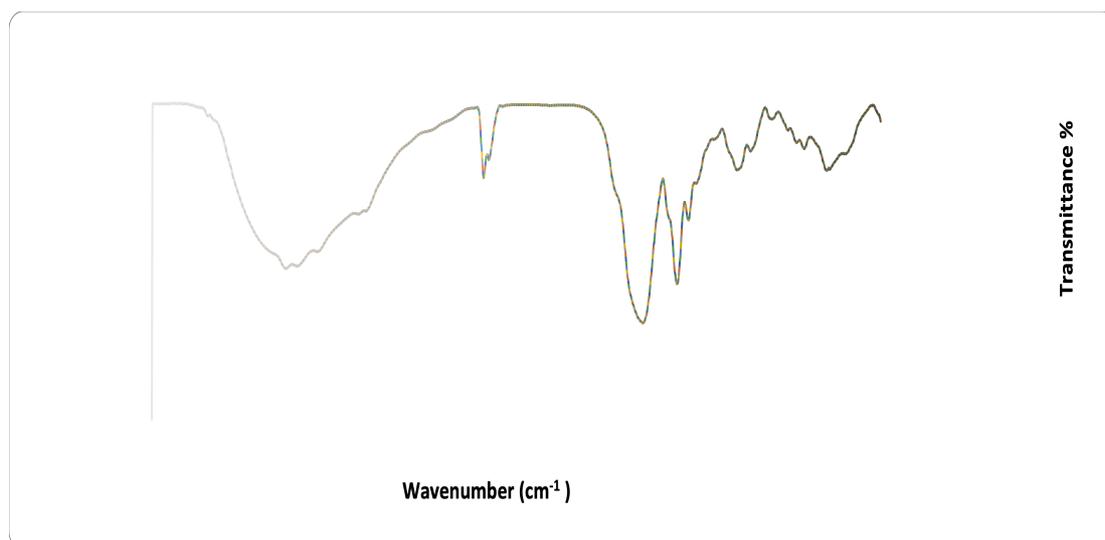
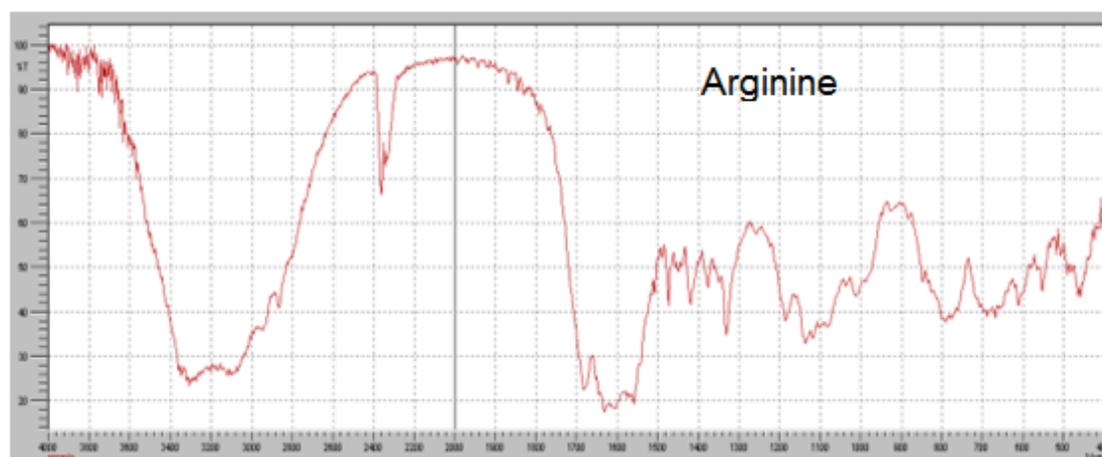
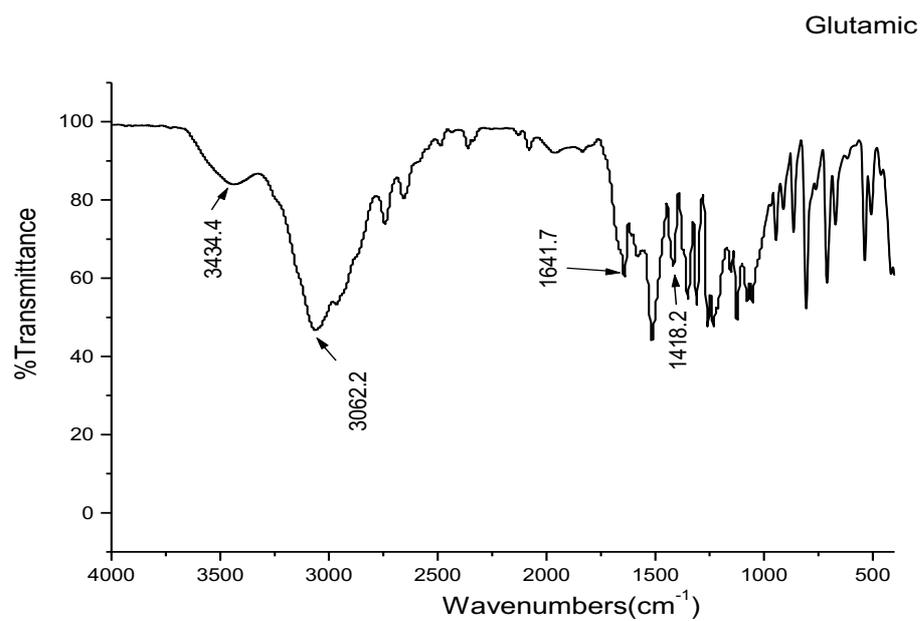


Figure 1S of Infrared spectra of glutamic, arginine and [Zn.Glu.Arg.(H₂O)₂].H₂O.

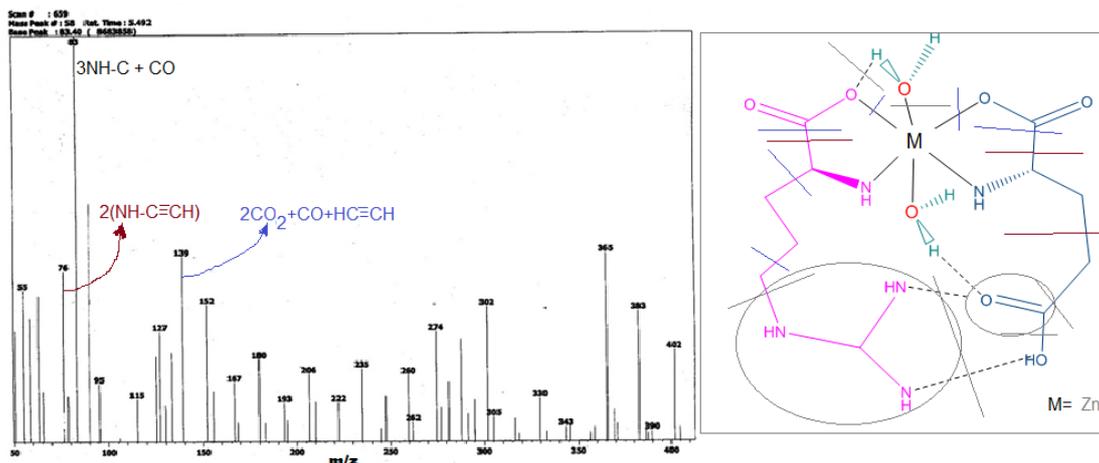


Fig 2S mass spectrum of Zn complex showing important fragments.

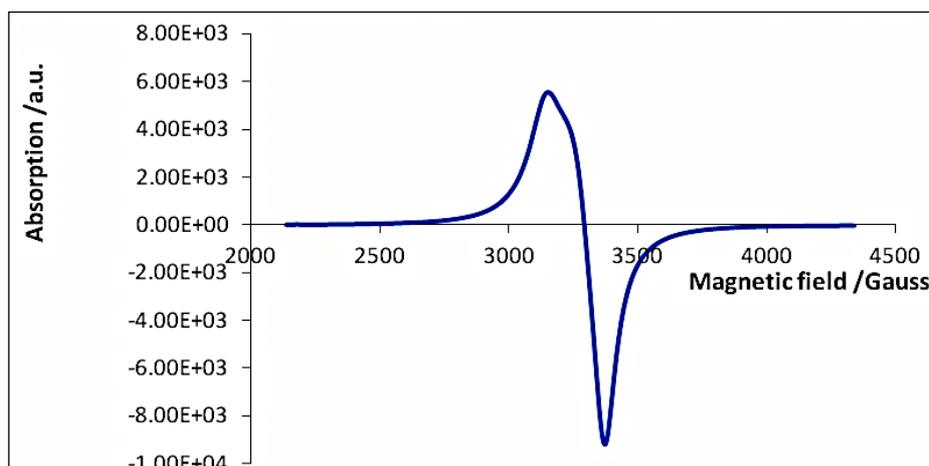


Fig 3S The EPR spectrum of the Cu(II)-complex (Similar spectrum is obtained in case of Co(II)-complex)

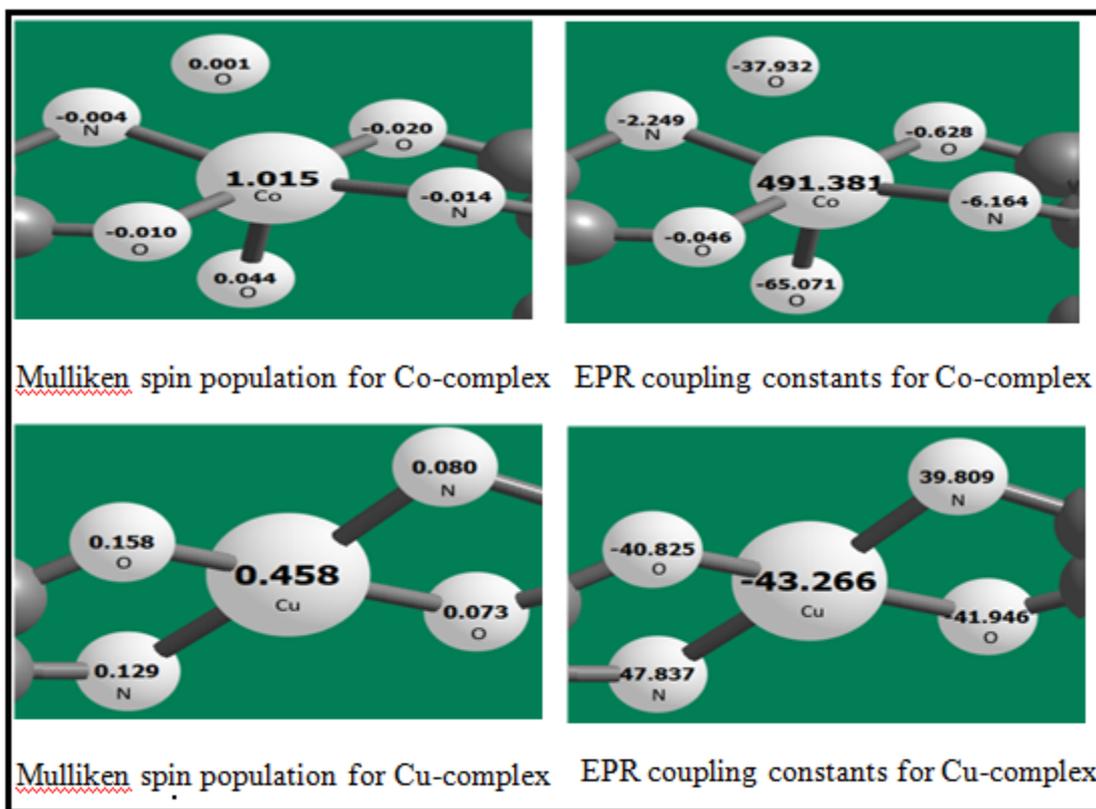


Fig 4S EPR Mulliken spin populations and Hyperfine (HF) coupling constants between Co(II)- and Cu(II)-ions bearing the unpaired electron and the surrounding O and N atoms of the chelates. HFC Values in MHz (1 MHz=0.00033356 cm⁻¹)

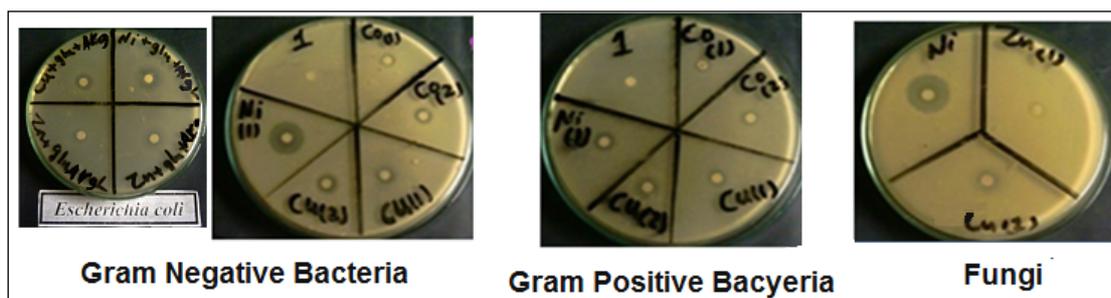


Fig 5S Some Photos of some microbial activity for the prepared complexes

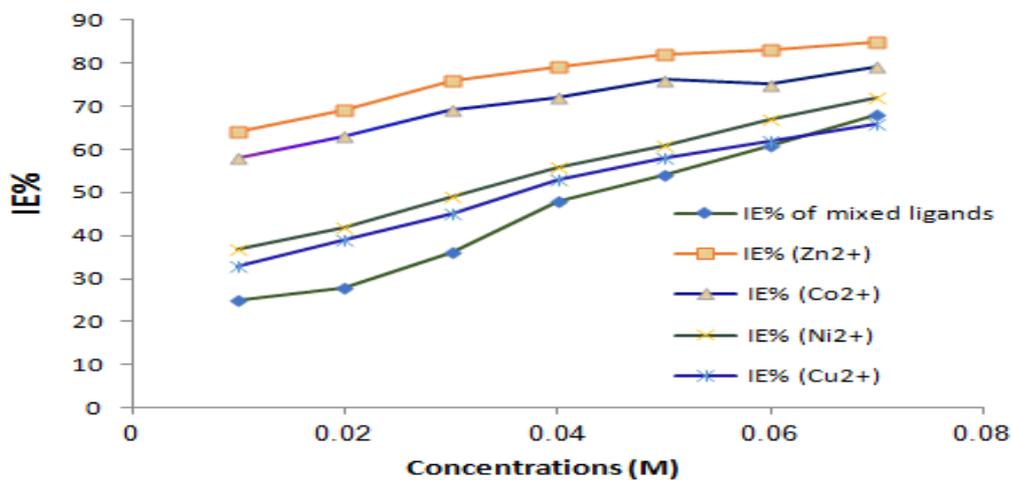


Fig 6S The inhibition efficiency of aluminum specimens in aqueous solution of 1M HCl with different concentrations of mixed ligands (glu.and arg.)and their ternary metal complexes at 303K for 7 h.

Table 1S MIP (molecular ion peak) values from mass spectra of the prepared complexes

Complex	MIP without outer sphere water	Molecular Mass
[Co(glu)(arg)(H ₂ O) ₂].H ₂ O	388.03 (Mt.Wt.-2H ₂ O=389.26)	425.26
[Ni(glu)(arg)(H ₂ O) ₂].0.5H ₂ O	386.71 (Mt.Wt.-2H ₂ O=389.03)	425.03
[Cu(glu)((arg)].H ₂ O	385.23 (Mt.Wt.-H ₂ O=384.87)	402.87
[Zn(glu)(arg)(H ₂ O) ₂].0.5H ₂ O	402.67 (Mt.Wt.-2H ₂ O=404.71)	440.71

Table 2S. Cytotoxicity evaluation of the ligands and their complexes

Complexes	IC₅₀, µg(HePG2)
[Glutamic]	43.7
[L-Arginine]	>50
[Co.Glu.Arg.(H ₂ O) ₂].0.5H ₂ O	15.4
[Ni.Glu.Arg.(H ₂ O) ₂].0.5H ₂ O	12.1
[Cu.Glu.Arg.].H ₂ O	8.6
[Zn.Glu.Arg.(H ₂ O) ₂].H ₂ O	11.8
Doxorubicin HCl	1.2