

Novel Thiazole–Phthalimide-Based Heterobimetallic Cu(II)-M(II) Complexes: Synthesis, Characterization, and Therapeutics Properties Against Arsenic-Induced Lung Damage in Rats

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Supplementary file

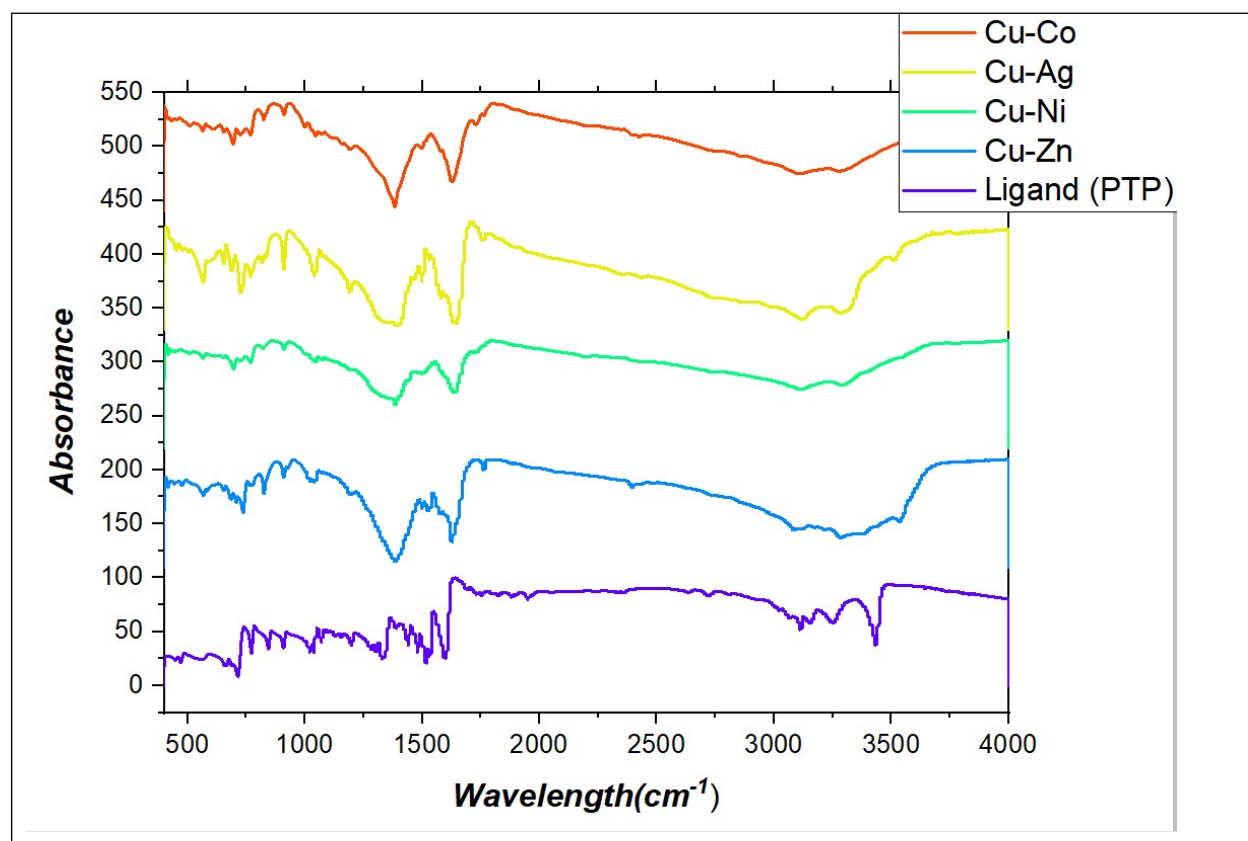


Figure S1. FT-IR spectra for PTP and its hetero-binuclear complexes

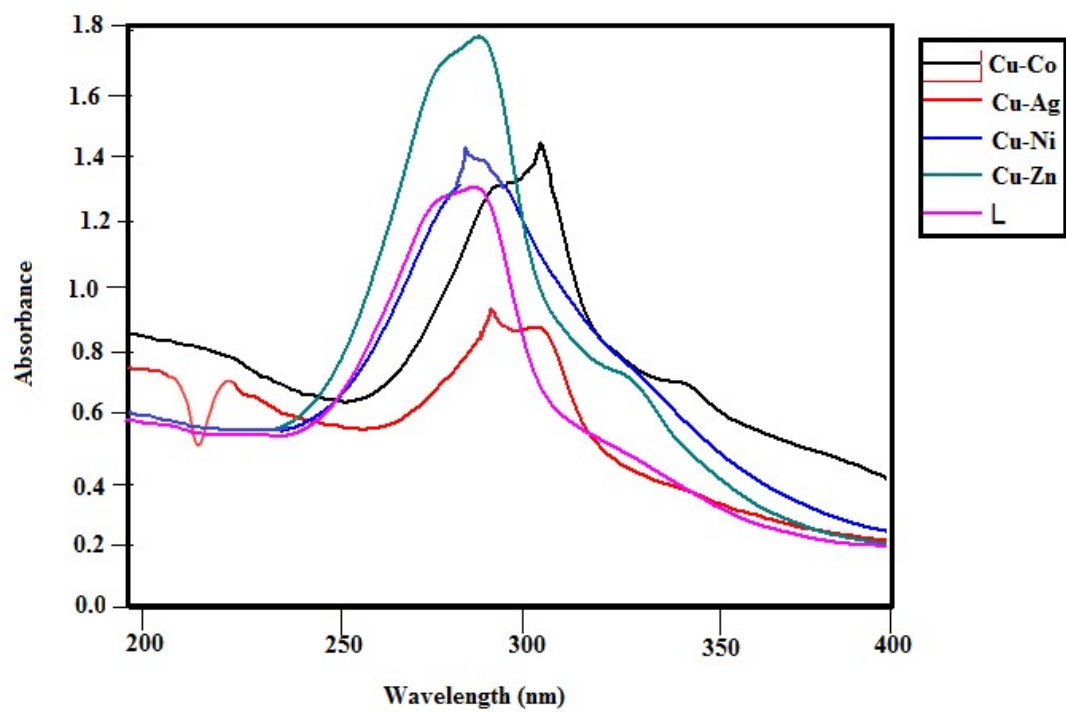


Figure S2: Electronic spectra of ligand and all metal complexes.

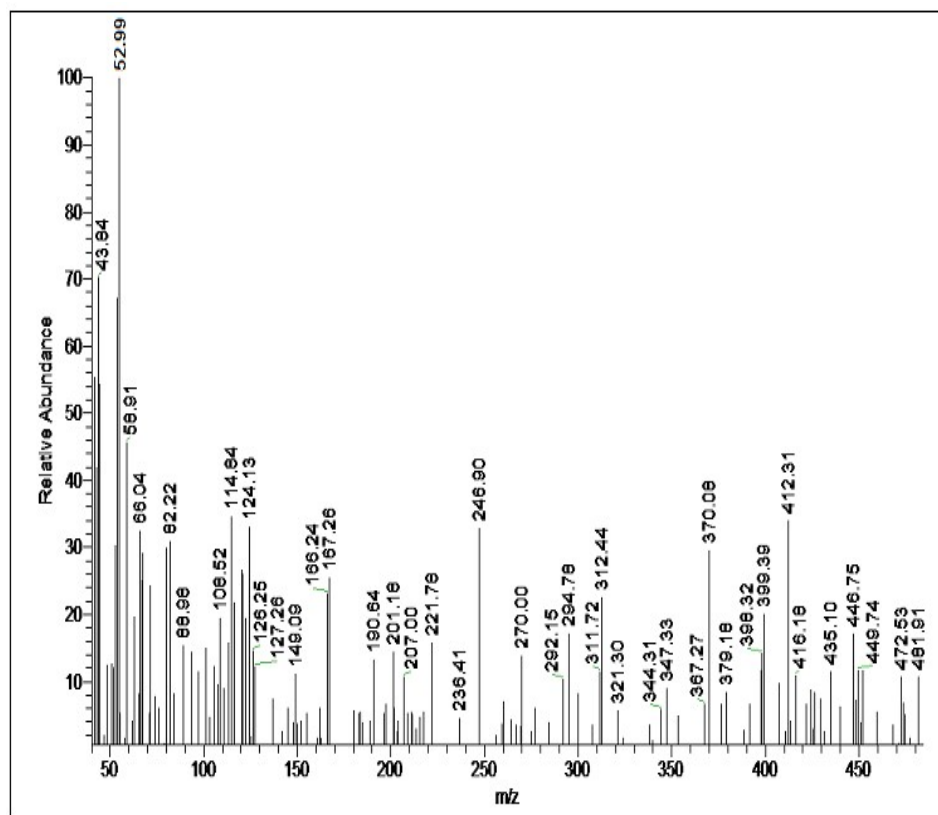


Figure S3. Mass spectrum of the PTP ligand.

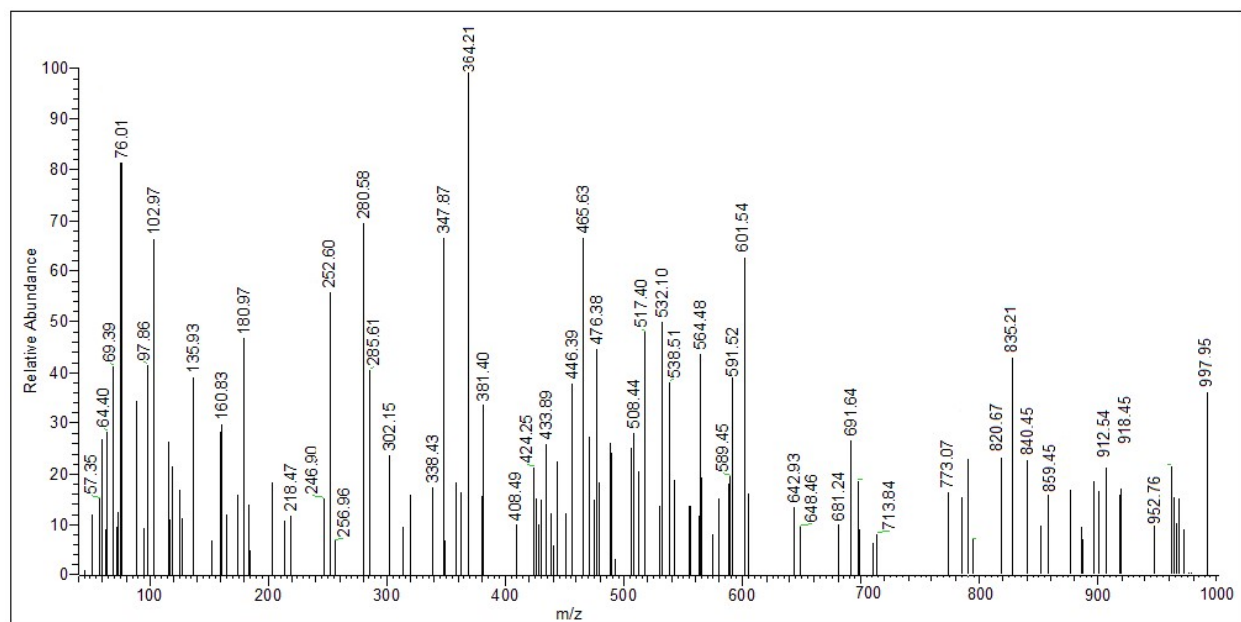


Figure S4. Mass spectrum of Cu-Co-PTP complex

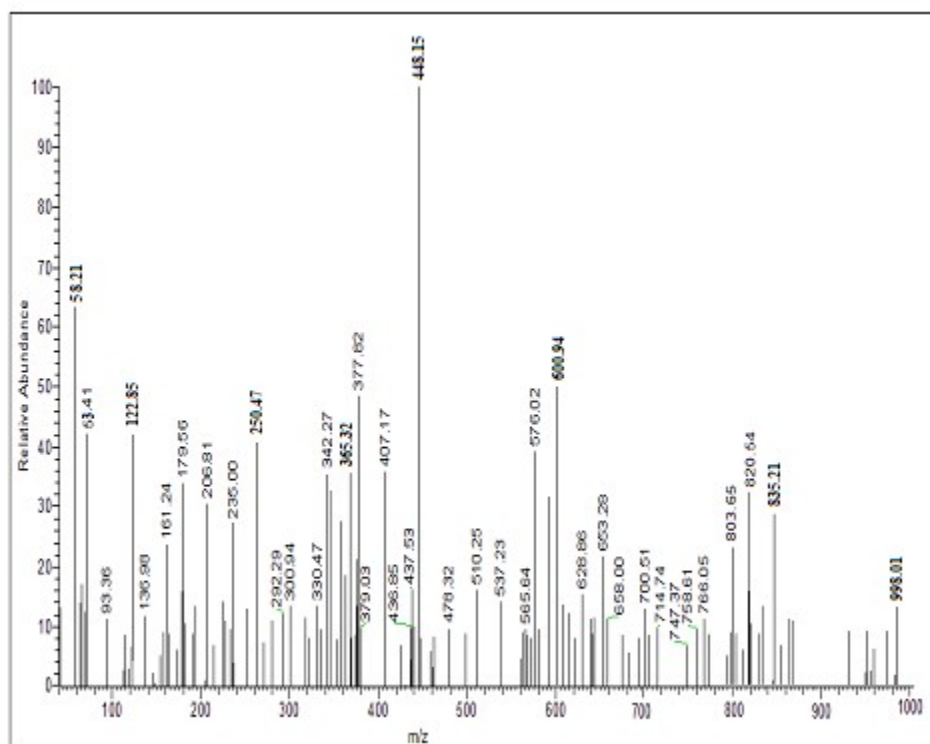


Figure S5. Mass spectrum of Cu-Ni-PTP complex

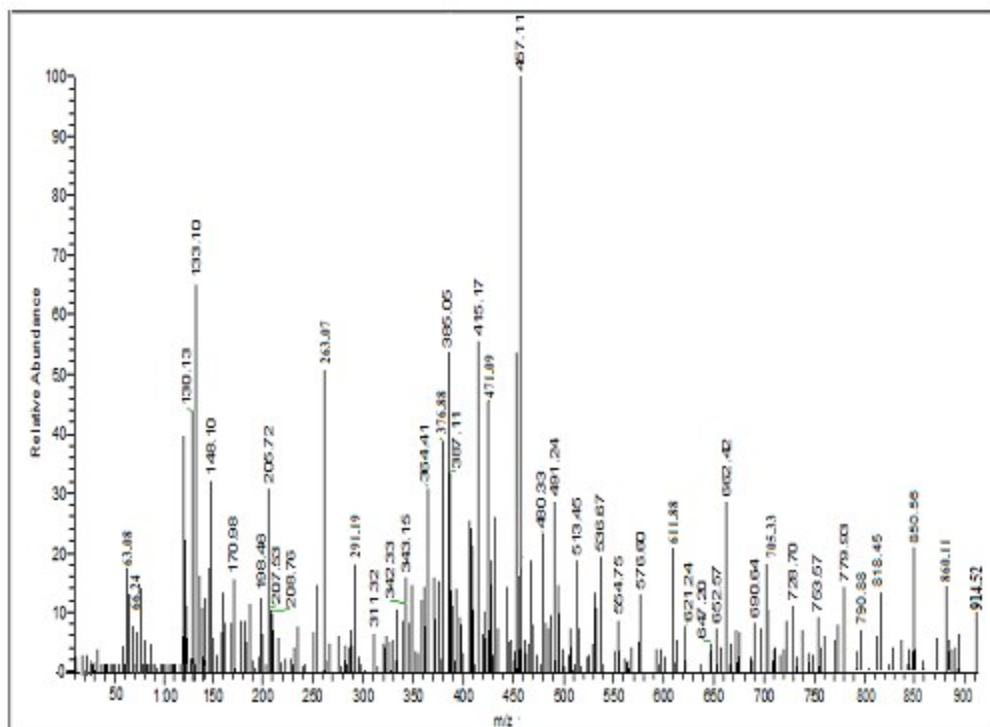


Figure S6. Mass spectrum of Cu-Zn-PTP complex

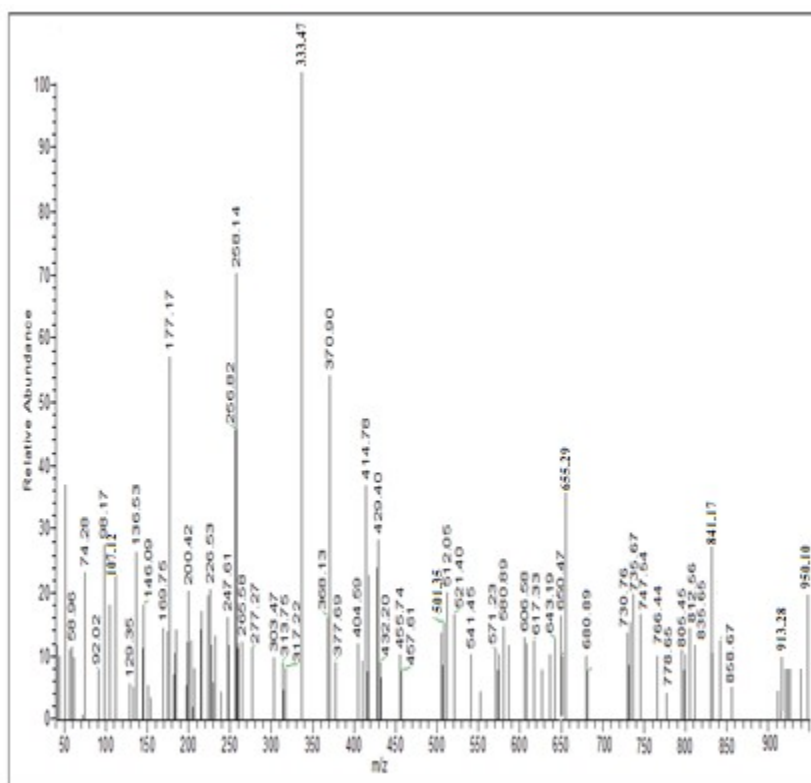


Figure S7. Mass spectrum of Cu-Ag-PTP complex

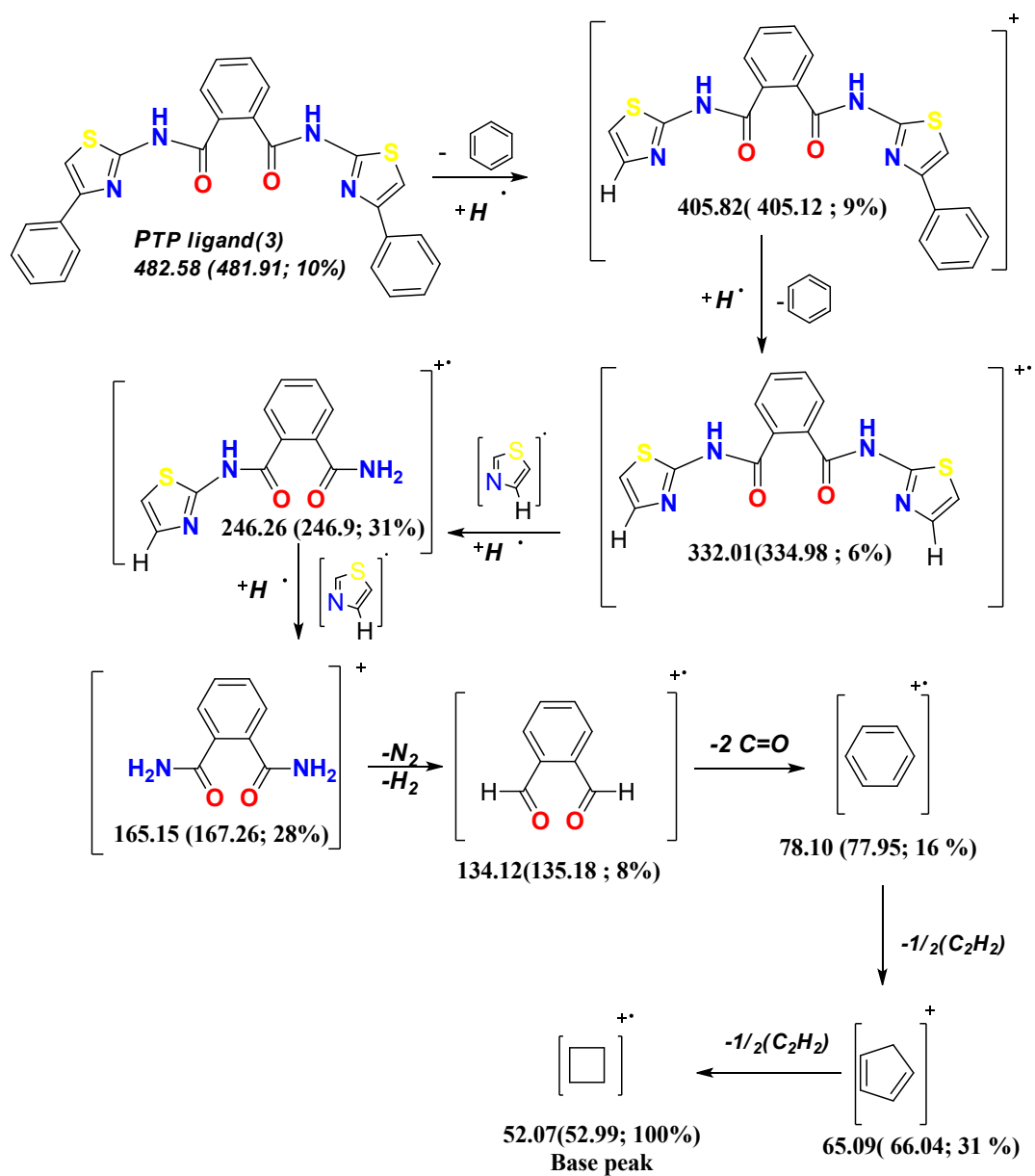


Figure S8. Mass fragmentation pattern of PTP, Calc. (Found, Relative intensity%), The loss or addition of H radicals causes differences between the computed and found values.

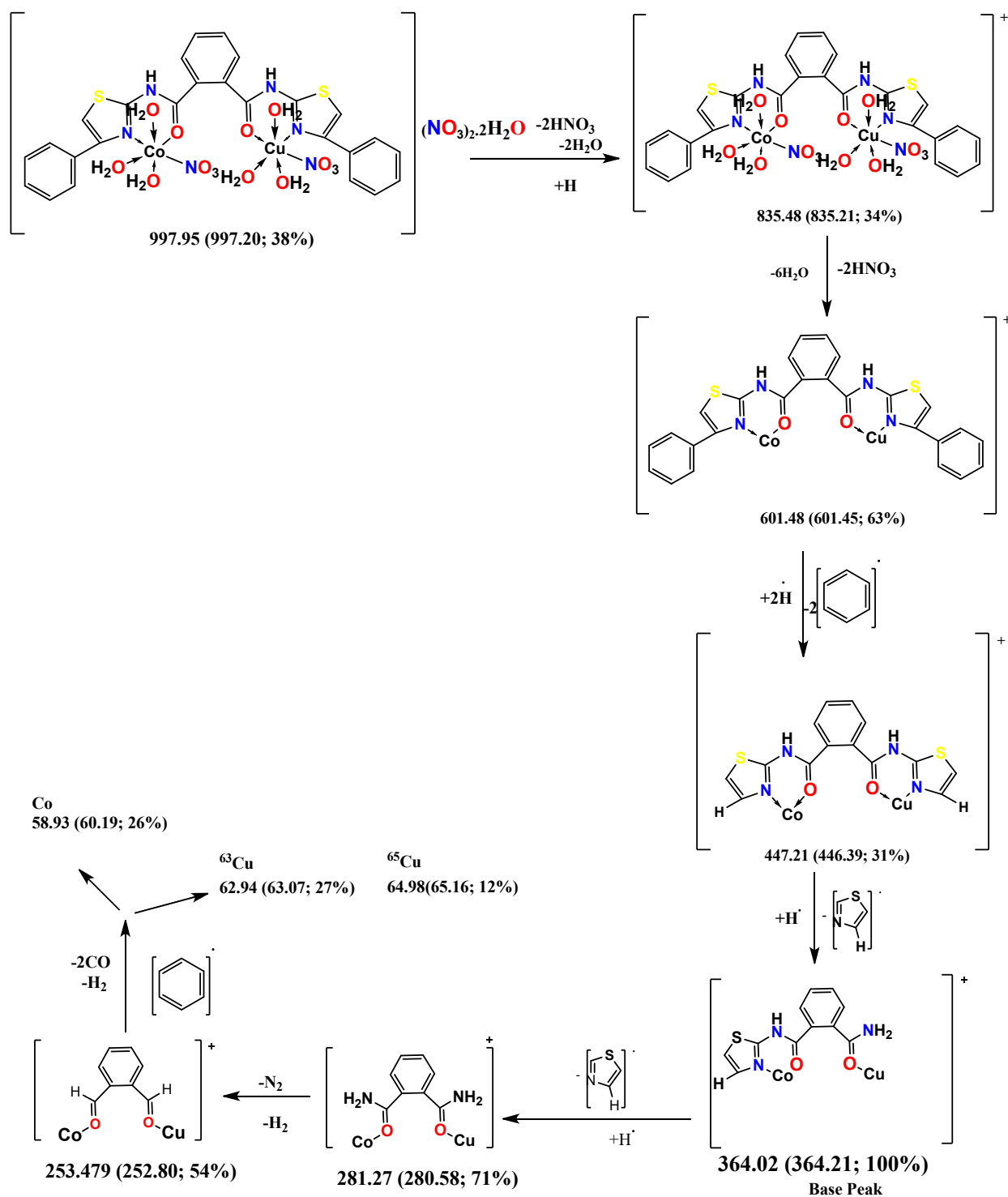


Figure S9: Mass fragmentation of Cu-Co-PTP complex

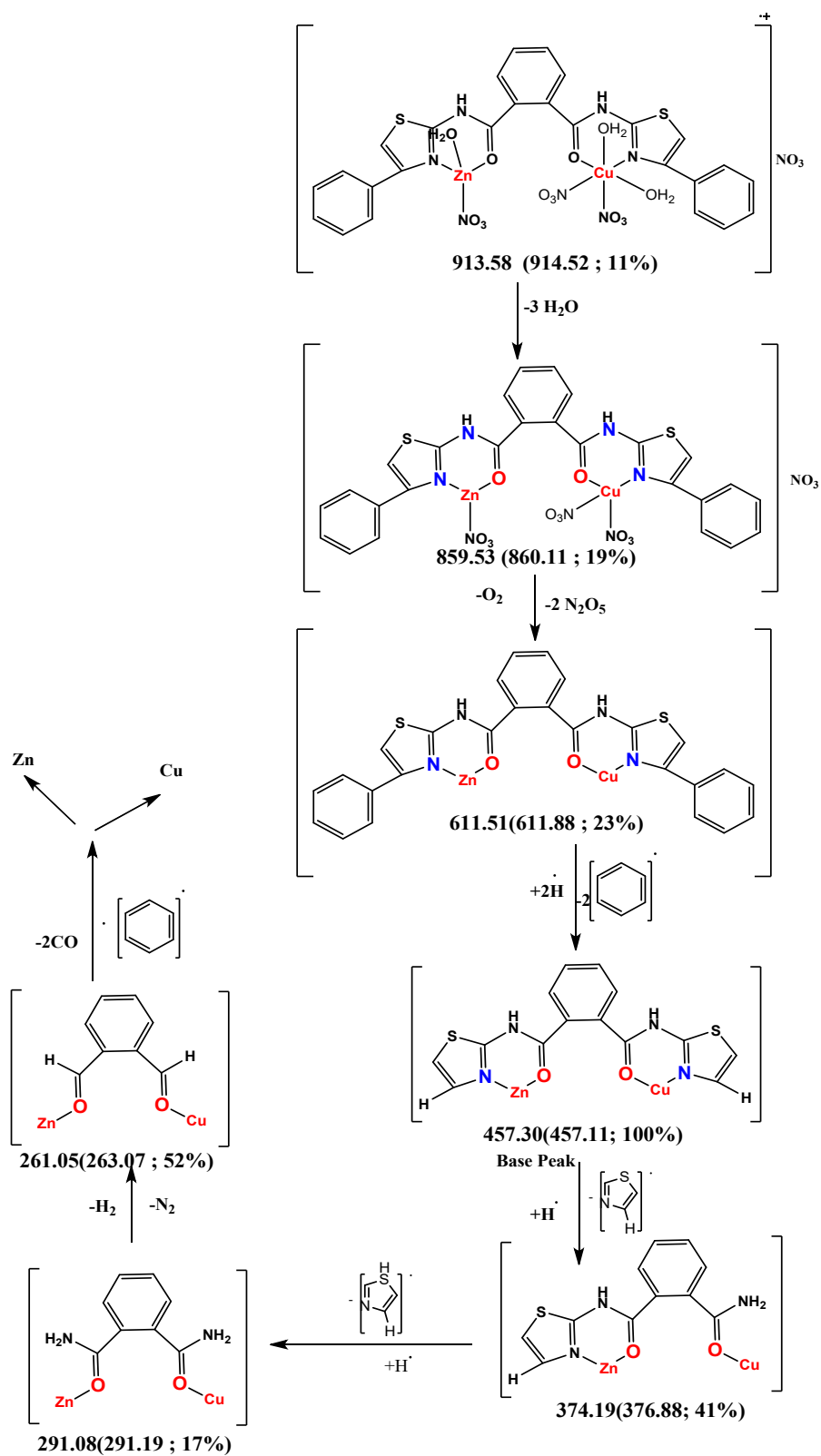


Figure S10: Mass fragmentation of Cu- Zn-PTP complex

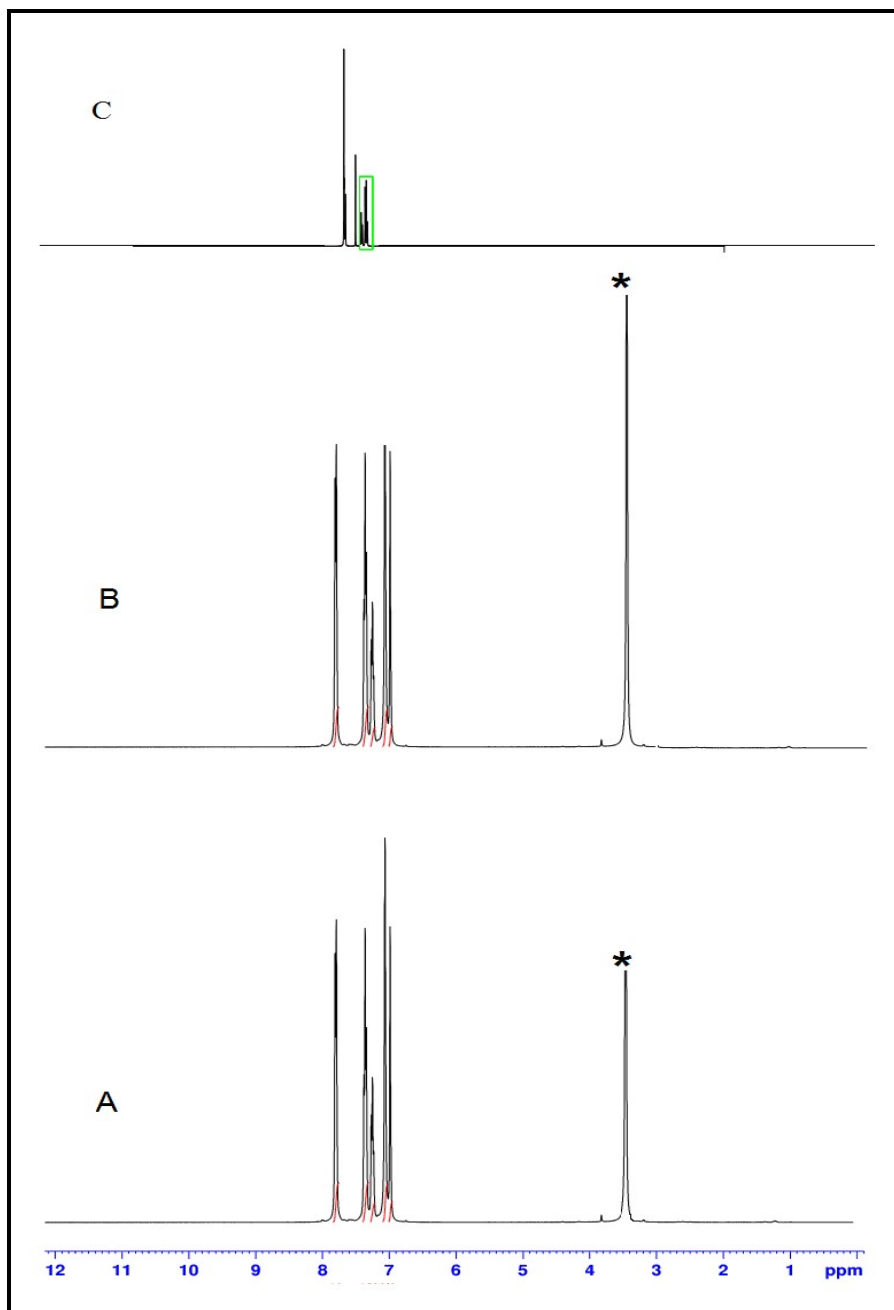


Figure S11. ^1H NMR spectra (δ , ppm.) in DMSO-d_6 solvent of (A) PTP ligand, (B) PTP ligand with D_2O and (C) theoretical data. Chemical shifts (ppm) were referenced externally at 25°C with respect to TMS, Asterisks (*) refer to suppressed solvent.

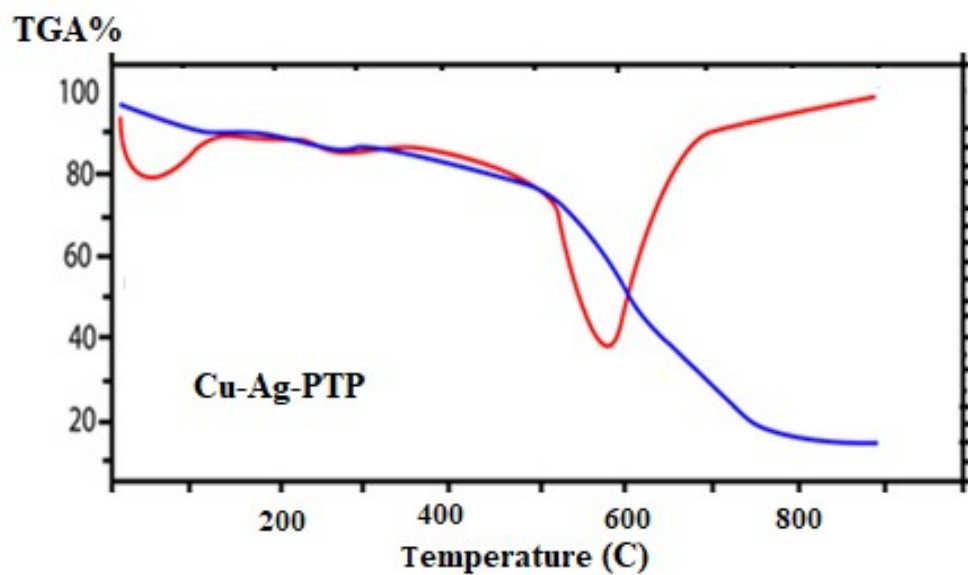
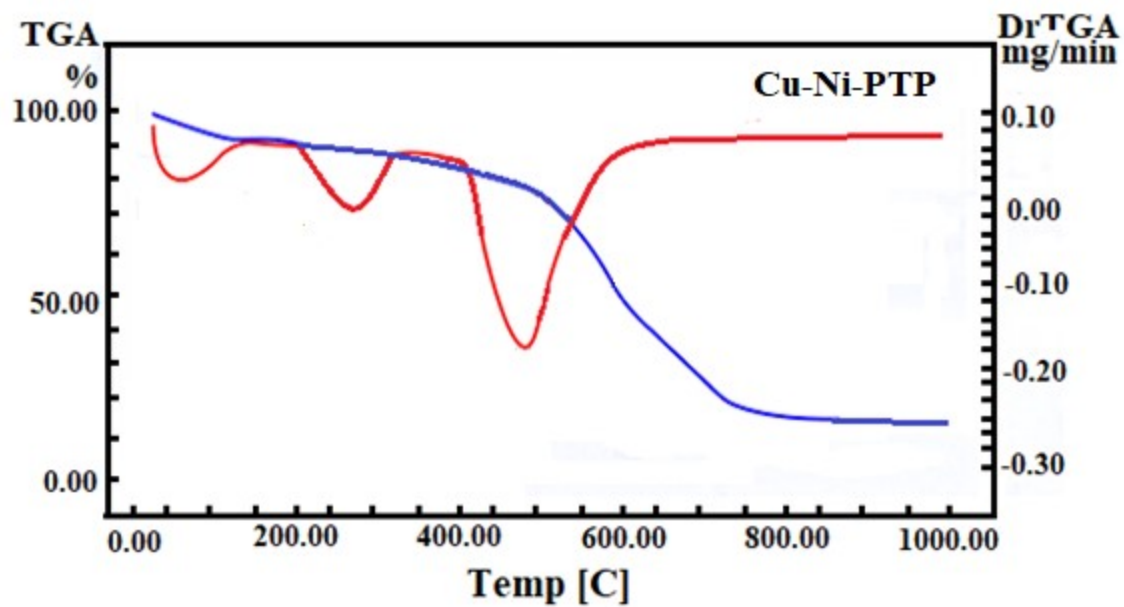


Figure S12. TGA for Cu-Ni-PTP and Cu-Ag-PTP complexes

Table S1. The obtained data of all substances:

<i>Compound</i>		<i>Molecular formula (M.Wt.)</i>	<i>Yield g; (%)</i>	<i>Color</i>	<i>Melting Point (°C)</i>	<i>Elemental analysis, Calc., (Found) (%)</i>			
						<i>C</i>	<i>H</i>	<i>N</i>	<i>S</i>
	<i>PTP complex</i>	C ₂₆ H ₁₈ N ₄ O ₂ S ₂ (482.58)	8.74 (80.00)	White	198-200	64.73 (64.74)	3.73 (3.72)	11.82 (11.84)	13.28 (13.26)
1	[CuCo(PTP)(NO ₃) ₂ (H ₂ O) ₆](NO ₃) ₂ .2H ₂ O Cu-Co-PTP	C ₂₆ H ₃₄ N ₈ O ₂₂ S ₂ CuCo (997.20)	4.56 (85.48)	Black	> 300	31.31 (31.32)	3.41 (3.40)	11.24 (11.23)	6.42 (6.41)
2	[CuNi(PTP)(NO ₃) ₂ (H ₂ O) ₆](NO ₃) ₂ .2H ₂ O Cu-Ni-PTP	C ₂₆ H ₃₄ N ₈ O ₂₂ S ₂ CuNi (996.96)	4.69 (87.79)	Greenish black	> 300	31.32 (31.31)	3.41 (3.42)	11.24 (11.25)	6.42 (6.41)
3	[CuZn(PTP)(NO ₃) ₃ (H ₂ O) ₃](NO ₃) Cu-Zn-PTP	C ₂₆ H ₂₄ N ₈ O ₁₇ S ₂ CuZn (913.58)	4.85 (90.32)	Dark brown	> 300	34.18 (34.17)	2.63 (2.64)	12.27 (12.35)	7.02 (7.00)
4	[CuAg(PTP)(NO ₃) ₂ (H ₂ O) ₄](NO ₃).2H ₂ O Cu-Ag-PTP	C ₂₆ H ₃₀ N ₇ O ₁₇ S ₂ CuAg (948.10)	4.42 (93.23)	Black	> 300	32.93 (32.94)	3.17 (3.18)	10.34 (10.33)	6.76 (6.75)

Table S2. Distinctive IR spectral assignment (cm⁻¹) of all compounds:

<i>Compound</i>	<i>ν(OH)</i>	<i>ν(NH)</i>	<i>ν(C=O)</i>	<i>ν(C=N) thiazole</i>	<i>ν(M-O)</i>	<i>ν(M-N)</i>
<i>PTP</i>		3294	1658	1613	...	
<i>Cu-Co-PTP</i>	3482-3120	3290	1645	1560	565	453
<i>Cu-Ni-PTP</i>	3436-3114	3289	1638	1580	566	451
<i>Cu-Zn-PTP</i>	3439 -3122	3291	1629	1574	567	476
<i>Cu-Ag-PTP</i>	3494-3123	3284	1632	1597	567	453

TableS3: Important mass data of synthesized heterobimetallic complexes.

Complex	Molar Mass	Important mass fragmentation (m/z) values
[Cu-Co-PTP]	(997.20)	997.95 (M), 835.21 (M- 2HNO ₃ + 2H ₂ O), 601.54 (loss of 2HNO ₃ , 6H ₂ O), 446.39 (loss of 2 phenyl of thiazole ring), 364.21 (loss of C ₃ HNS), 280.58 (loss of C ₃ HNS), 252.60 (loss of N ₂ +H ₂), 180.97 (loss of phenyl ring), 150.74 (loss of 2CO)
Cu-Ni-PTP	(996.96)	998.01 (M), 835.21 (loss of 2HNO ₃ +2H ₂ O), 600.94 (Loss of 2HNO ₃ +6H ₂ O), 447.58 (Loss of 2 phenyl of thiazole ring), 280.35 (loss of 2C ₃ HNS), 250.47 (loss of N ₂ +H ₂), 121(loss of phenyl ring +2CO)
Cu-Zn-PTP	(913.58)	914.52 (M), 860.11 (loss of 2H ₂ O), 611.88 (loss of 2N ₂ O ₅ +O ₂), 457.11(loss of 2 phenyl of thiazole ring), 376.88 (loss of C ₃ HNS), 291.19 (loss of C ₃ HNS), 263.07 (loss of N ₂ +H ₂), 128.85 (loss of phenyl ring+ 2CO)

Cu-Ag-PTP	(948.10)	950.12 (M+2), 913.28 (loss of 2H ₂ O), 841.17(loss of 4H ₂ O), 655.29 (loss of N ₂ O ₅ + NO ₂ +O ₂), 503.53 (loss of 2 phenyl of thiazole ring), 333.47 (loss of 2C ₃ HNS), 303.47 (loss of N ₂ +H ₂), 171.52 (loss of phenyl ring+ 2CO)
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Table S4: Thermoanalytical results (TGA-DTG) for all metal complexes.

Complexes	Stage	ΔT (°C)	Weight Loss (%)		Assignment	Metals oxide (%)	
			Obsd.	Calcd.		Obsd.	Calcd.
Cu-Co	1 st	(46-224°C)	15.129	14.451	Loss of 2 uncoordinated H ₂ O, 6 coordinated H ₂ O molecules	14.576	15.502
	2 nd	(225-490°C)	30.043	29.404	Loss of 2N ₂ O ₅ molecule, phenyl ring of thiazole moiety.		
	3 rd	(491-800°C)	40.252	40.643	Loss of the remaining organic ligand.		
Cu-Ni	1 st	(79-198°C)	15.123	14.454	Loss of 2 uncoordinated H ₂ O, 6 coordinated H ₂ O molecules	15.038	15.482
	2 nd	(199-470°C)	37.025	37.139	Loss of 2N ₂ O ₅ molecule, 2phenyl rings of thiazole moiety.		
	3 rd	(471-800°C)	32.814	32.925	Loss of the remaining organic ligand.		
Cu-Zn	1 st	(201-495°C)	55.499	55.578	Loss of 3 coordinated H ₂ O molecules, 2N ₂ O ₅ molecules, 2 phenyl rings of thiazole moiety, C ₃ HNS	18.580	17.351
	2 nd	(496-800°C)	25.921	26.865	Loss of the remaining organic ligand		
Cu-Ag	1 st	(82-450°C)	27.858	27.648	Loss of 2 uncoordinated H ₂ O, 4 coordinated H ₂ O molecules, N ₂ O ₅ molecule, NO ₂ molecule	20.972	19.769
	2 nd	(451-675°C)	20.111	19.642	Loss of phenyl ring of thiazole moiety, O ₂ molecule		
	3 rd	(676-800°C)	31.059	31.263	Loss of the remaining organic ligand.		