

Supporting Information

Insighting the Inhibitory Potential of Metal Complexes Supported by (*E*)-2-Morpholino-*N*-(thiophen-2-ylmethylene)ethanamine: Synthesis, Structural Properties, Biological Evaluation and Docking Studies

Saira Nayab,^{a,f} Kalsoom Jan,^{b,c} Seung-Hyeon Kim,^d Sa-Hyun Kim,^d Dilawar Farhan

Shams,^e Younghu Son,^f Minyoung Yoon,^{f,*} and Hyosun Lee,^{f,*}

^a Department of Chemistry, Shaheed Benazir Bhutto University, Sheringal Dir (U) 18050, Khyber Pakhtunkhwa, Islamic Republic of Pakistan

^b Department of Plastics Engineering, University of Massachusetts Lowell, Lowell, MA 01851 USA

^c Department of Chemistry, University of Massachusetts Lowell, Lowell, MA 01851 USA.

^d BK21 FOUR KNU Creative BioResearch Group, School of Life Science, Kyungpook National University, 80 Daehakro, Bukgu, Daegu, 41566, Republic of Korea.

^e Department of Environmental Chemistry, Abdul Wali Khan University Maradan, Khyber Pakhtunkhwa, Islamic Republic of Pakistan

^f Department of Chemistry and Green-Nano Materials Research Center, Kyungpook National University, 80 Daehakro, Bukgu, Daegu, 41566, Republic of Korea

***CORRESPONDING AUTHORS**

Prof. Minyoung Yoon E-mail: myyoon@knu.ac.kr

Prof. Hyosun Lee E-mail: hyosunlee@knu.ac.kr

Time (sec)	3.2768	Comment	TEM ligand	Date	02 Mar 2022 14:11:12
C:\Users\jpr\Desktop\Sara Data\Sara NMR\TEM Ligand and Zn, Cd complexes (DMSO)\TEM ligand (DMSO)\pdata1\11r					
MHz	500.15	Nucleus	¹ H	Number of Transients	16
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in	50.80	SW(Cyclical) (Hz)	10000.00	Solvent	DMSO-d6
type	STANDARD	Sweep Width (Hz)	9999.85	Temperature (degree C)	22.800
				Origin	spect
				Pulse Sequence	zg30
				Spectrum Offset (Hz)	3982.9954

ligand (DMSO) 001 1r Vertical Scale Factor = 1

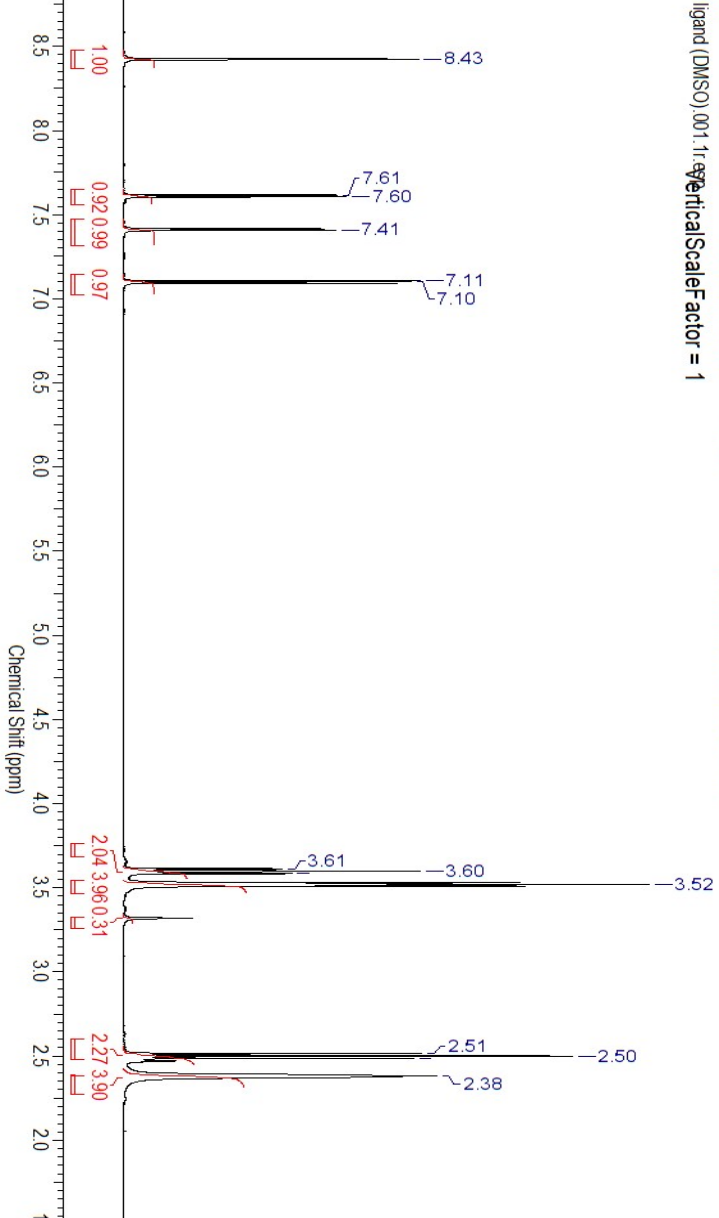


FIGURE S1. ¹H NMR spectrum of TEM.

This report was created by ACQ/NMR Processor Academic Edition. For more information go to www.acdlabs.com/nmrprocl/

6/7/2022 12:00:51 PM

Acquisition Time (sec)	1.1010	Comment	TEM	Date	27 May 2022 22:26:24	Date Stamp	27 May 2022 22:26:24
File Name	C:\Users\pro\Desktop\20-26\TEM-C NMR\PDAT\1\1\			Frequency (MHz)	125.76	Nucleus	¹³ C
Origin	spect	Original Points Count	32768	Owner	nm-500	Points Count	32768
Receiver Gain	2060.00	SW (cyclical) (Hz)	29761.90	Solvent	DMSO-d6	Spectrum Offset (Hz)	12576.8057
Preamp Width (Hz)	29761.00	Temperature (degree C)	25.300			Pulse Sequence	zpgq30
						Spectrum Type	STANDARD

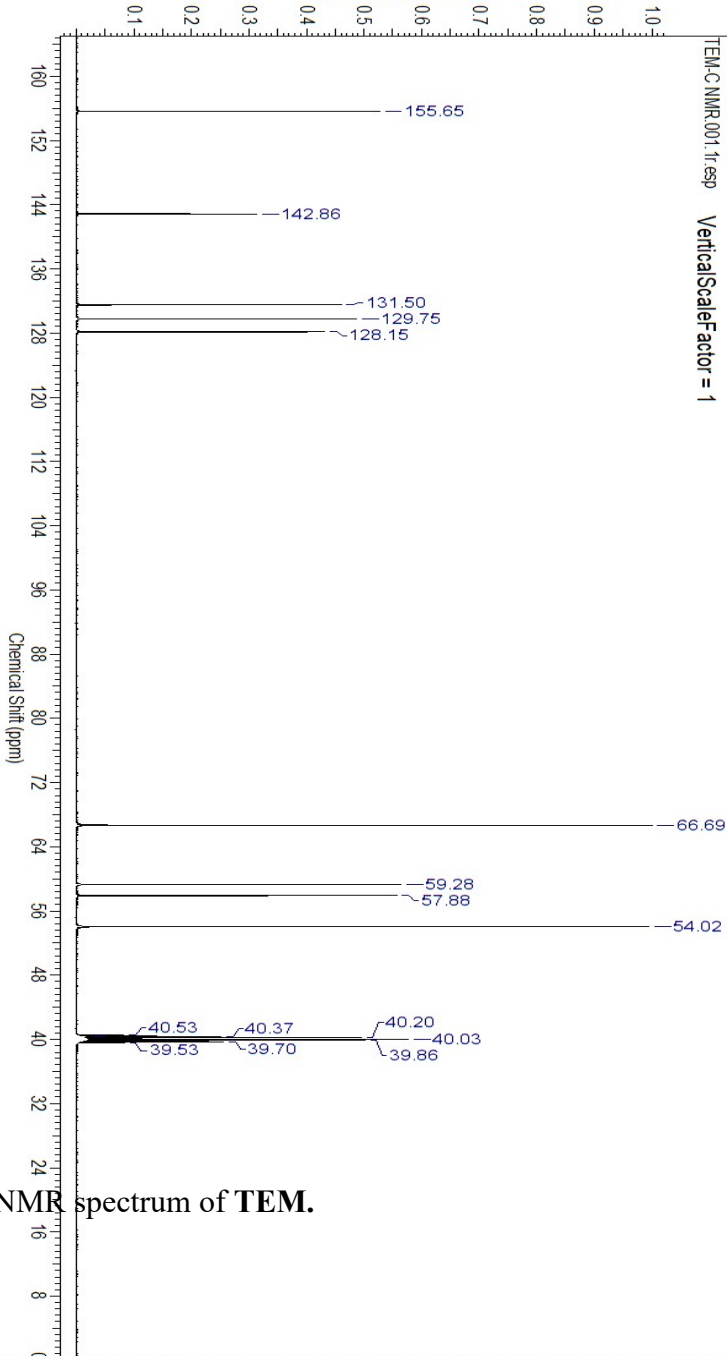


FIGURE S2. ¹³C NMR spectrum of TEM.

Acquisition Time (sec)	3.2768	Comment	TEM_Zn	Date	02 Mar 2022 14:15:28
Date Stamp	02 Mar 2022 14:15:28				
File Name	C:\Users\pro\Desktop\Sara Data\Sara NMR\TEM Ligand and Zn_Cd complexes (DMSO)\TEM_Zn (DMSO)\pdata11r				
Frequency (MHz)	500.15	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Owner	nm500	Points Count	65536
Receiver Gain	287.00	SW(cyclical) (Hz)	10000.00	Solvent	DMSO-d6
Spectrum Type	STANDARD	Sweep Width (Hz)	9999.85	Temperature (degree C)	22.800

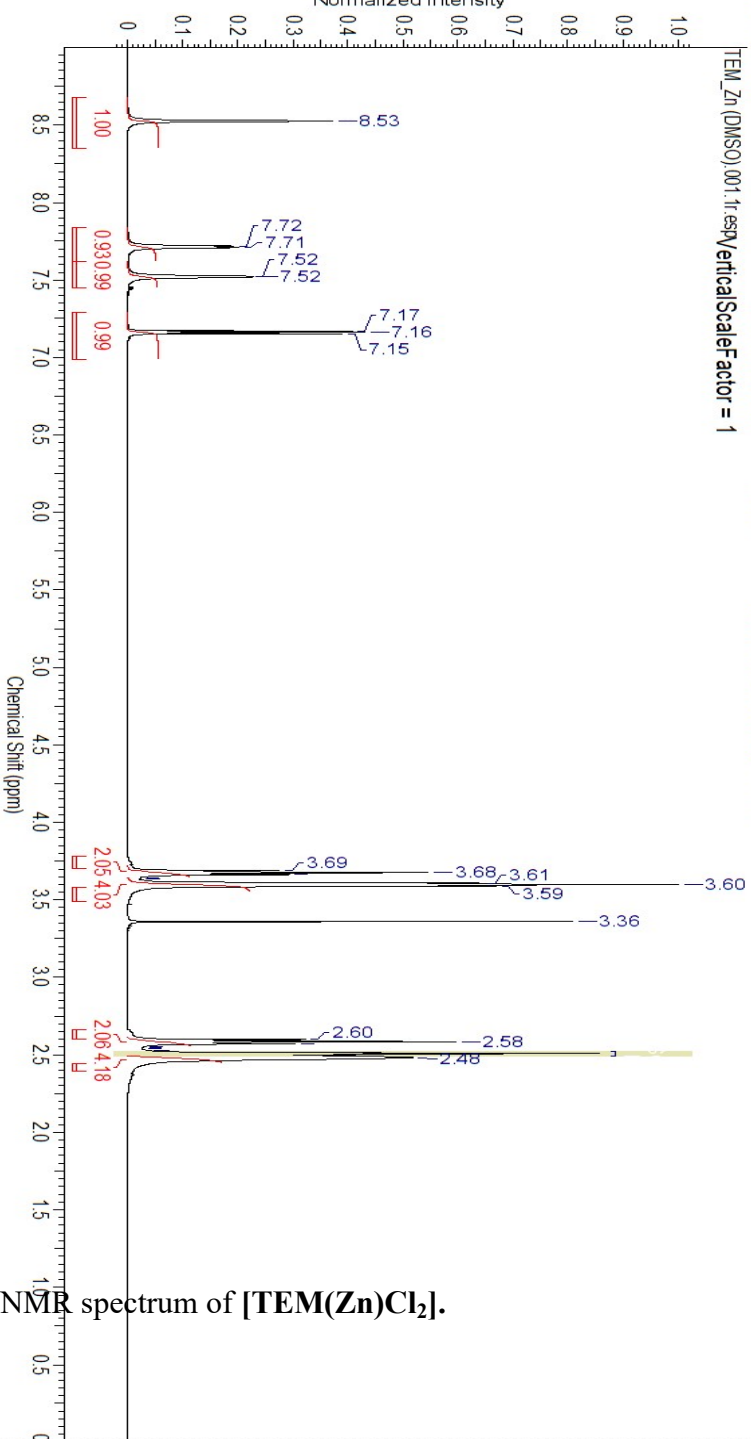


FIGURE S3. ¹H NMR spectrum of [TEM(Zn)Cl₂].

Acquisition Time (sec)	3.2768	Comment	TEM-Cd	Date	02 Mar 2022 14:21:52
File Stamp	02 Mar 2022 14:21:52				
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Frequency (MHz)	500.15	Nucleus	¹ H	Number of Transients	16
Original Points Count	32768	Owner	nm500	Points Count	65536
Receiver Gain	287.00	SW (cyclic) (Hz)	10000.00	Solvent	DMSO-d6
Spectrum Type	STANDARD	Sweep Width (Hz)	9999.85	Temperature (degree C)	22.800
				Origin	spect
				Pulse Sequence	zg30
				Spectrum Offset (Hz)	4001.1992

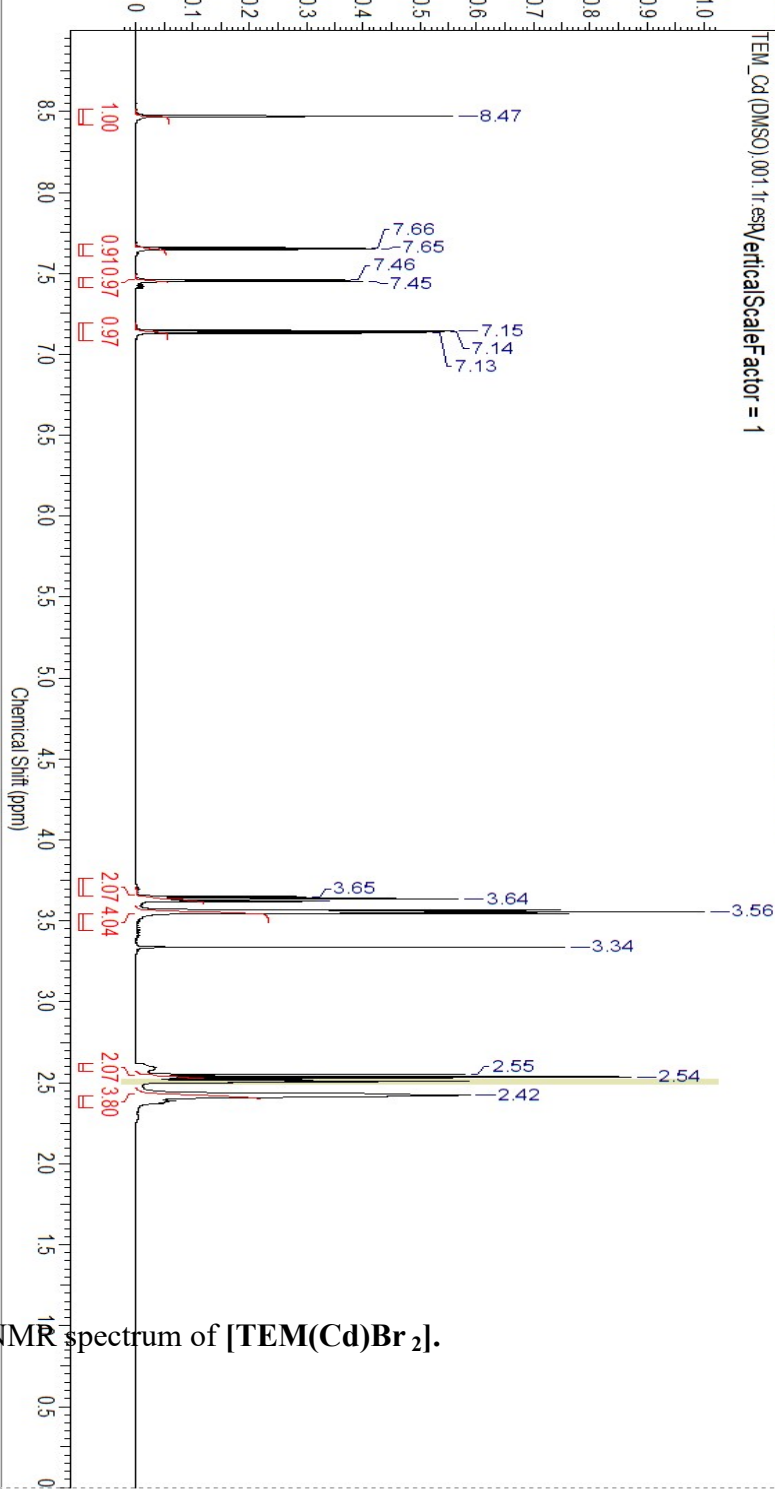


FIGURE S4. ¹H NMR spectrum of [TEM(Cd)Br₂].

Sample Name	18 Jul 2022 17:14:56	Comment	TEM-Zn	Date	18 Jul 2022 17:14:56
File Path	C:\Users\pro\Desktop\Saira Data\Saira NMR\TEM Ligand and Zn_Cd complexes (DMSO)\TEM-Zn (DMSO4) C NMR Corrected\PDAT\11r				
Frequency (MHz)	125.76	Nucleus	¹³ C	Number of Transients	2048
Points Count	32768	Owner	nm500	Points Count	32768
Power Gain	2050.00	SW (cyclical) (Hz)	29761.90	Solvent	DMSO-d6
Scan Type	STANDARD	Sweep Width (Hz)	29761.00	Temperature (degree C)	26.400

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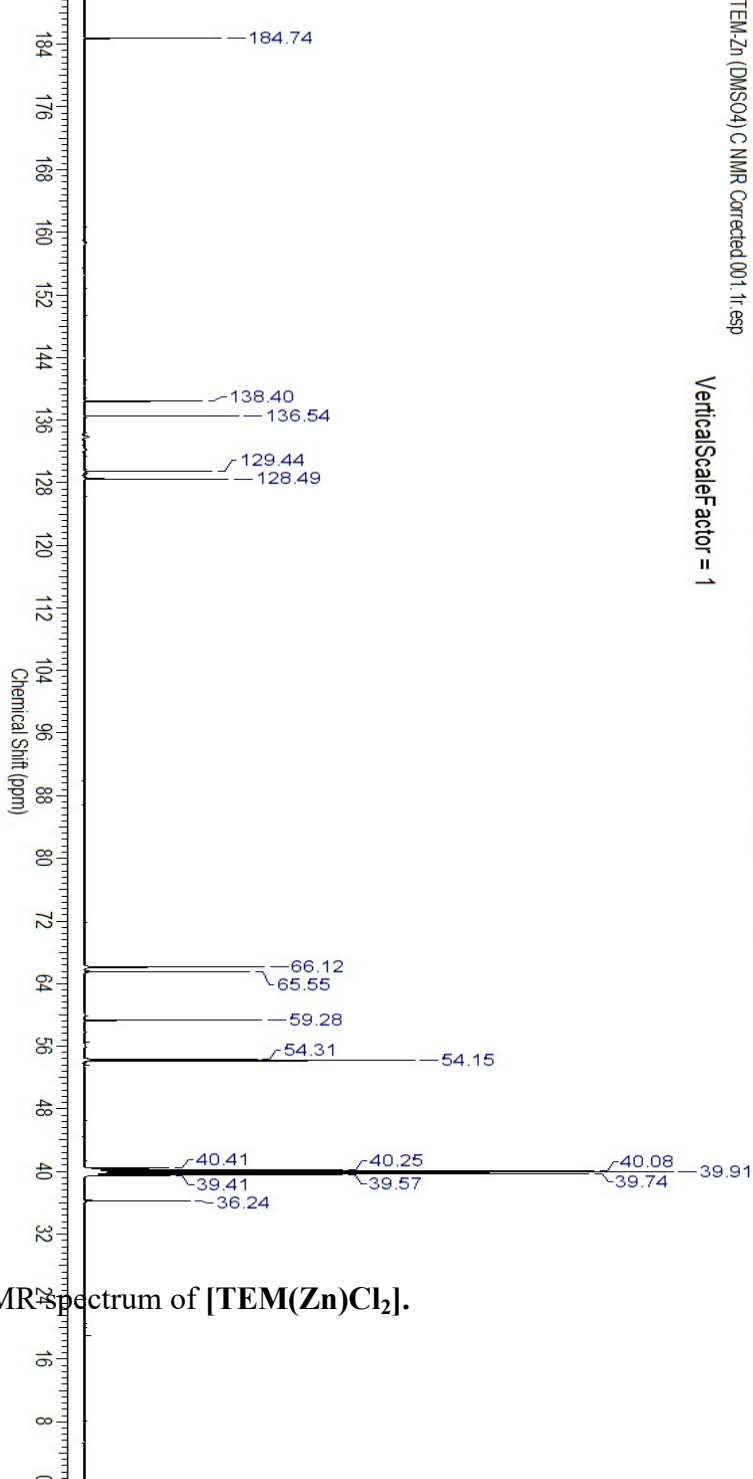


FIGURE S5. ¹³C NMR spectrum of [TEM(Zn)Cl₂].

Acquisition Time (sec)	1.1010	Comment	TEM-Cd	Date	28 May 2022 02:10:24
Date Stamp	28 May 2022 02:10:24	Nucleus	¹³ C	File Name	C:\Users\jpro\Desktop\20-26\TEM-Cd C NMR\PPDA\TA\11r
Frequency (MHz)	125.76	Points Count	32768	Number of Transients	2048
Owner	nm500	Spectrum Offset (Hz)	125768057	Pulse Sequence	zgpg30
Solvent	DMSO-d6	Spectrum Type	STANDARD	Receiver Gain	2050.00
				Sweep Width (Hz)	29761.00
				Original Points Count	32768
				SW (cycles) (Hz)	29761.90
				Temperature (degree C)	25.400

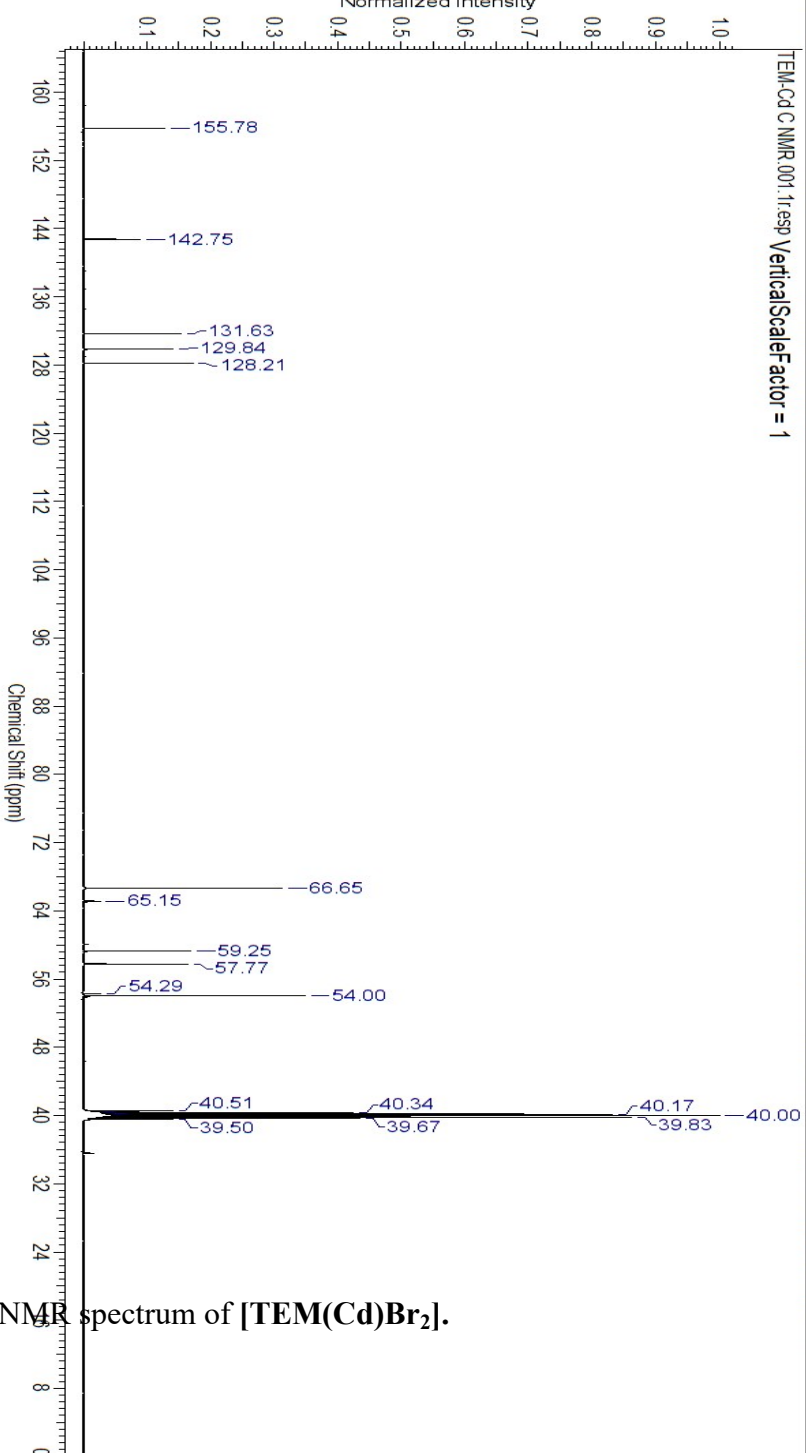


FIGURE S6. ¹³C NMR spectrum of [TEM(Cd)Br₂].

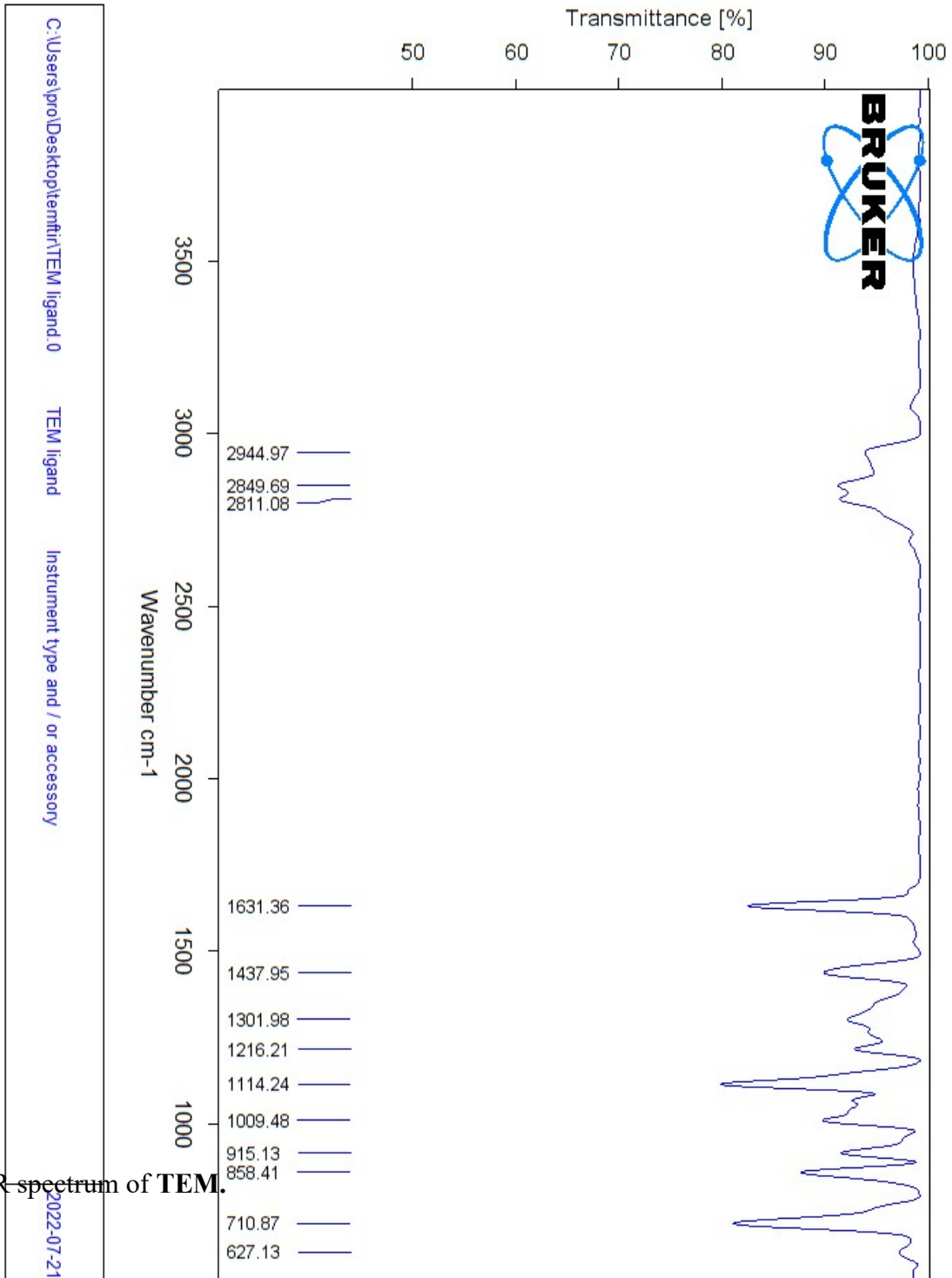


FIGURE S7. FTIR-spectrum of TEM.

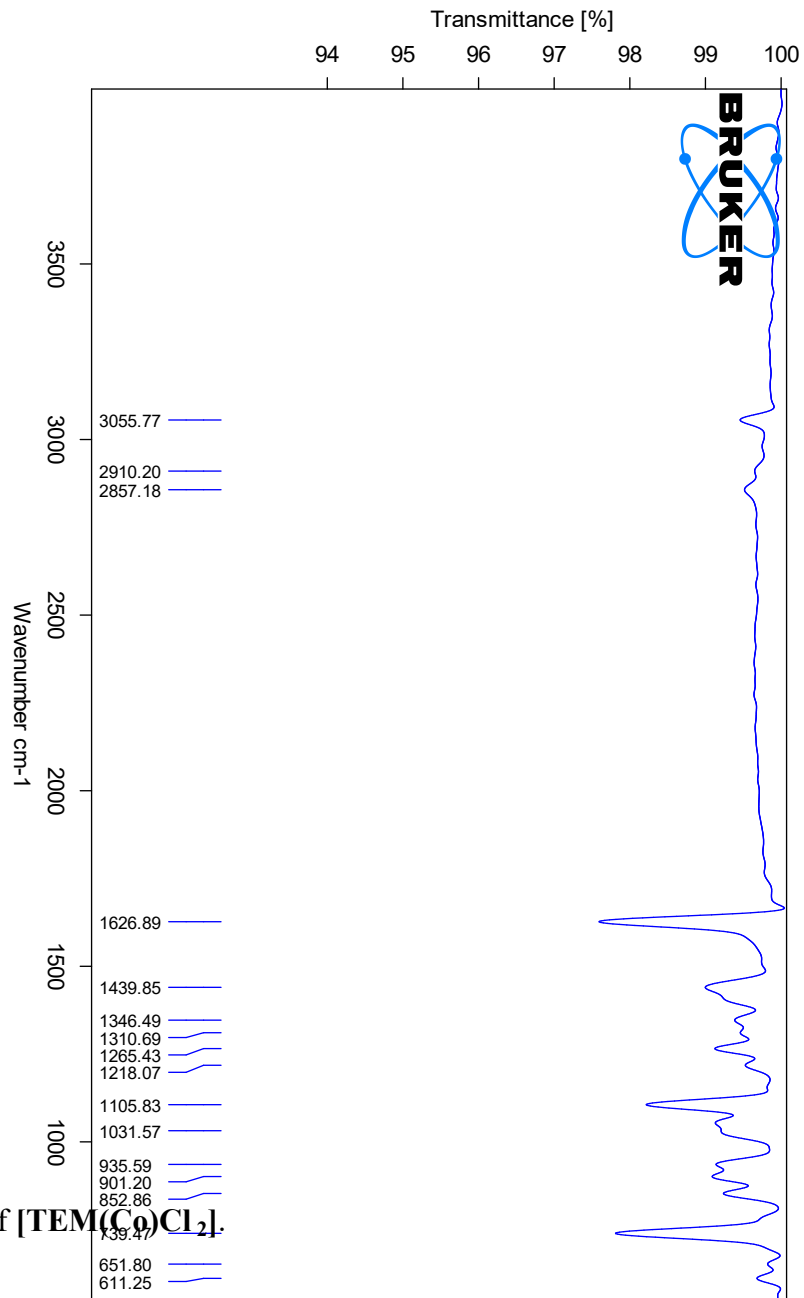


FIGURE S8. FTIR spectrum of [TEM(CO)Cl₂].

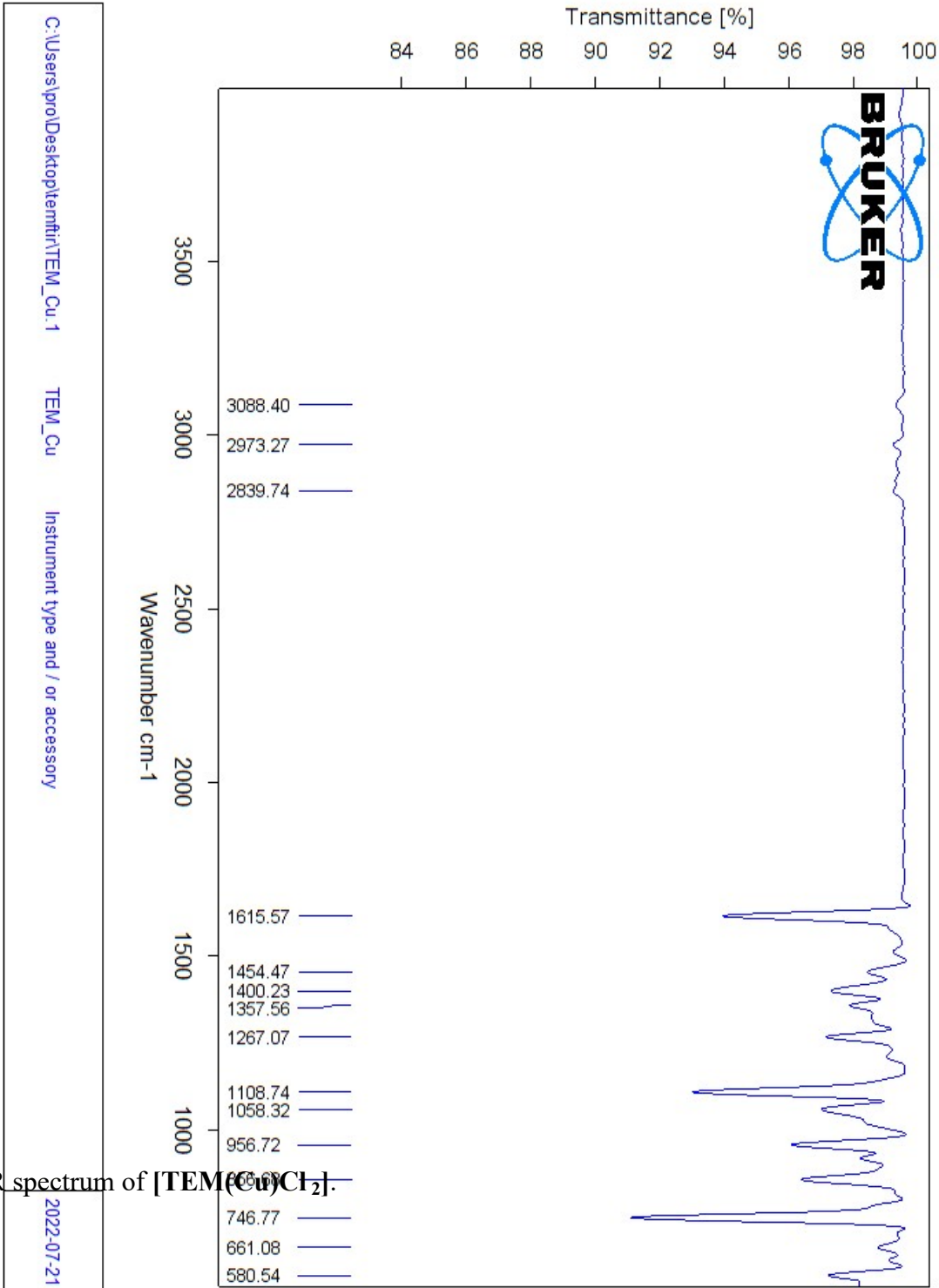


FIGURE S9. FTIR spectrum of [TEM(Cu)Cl₂].

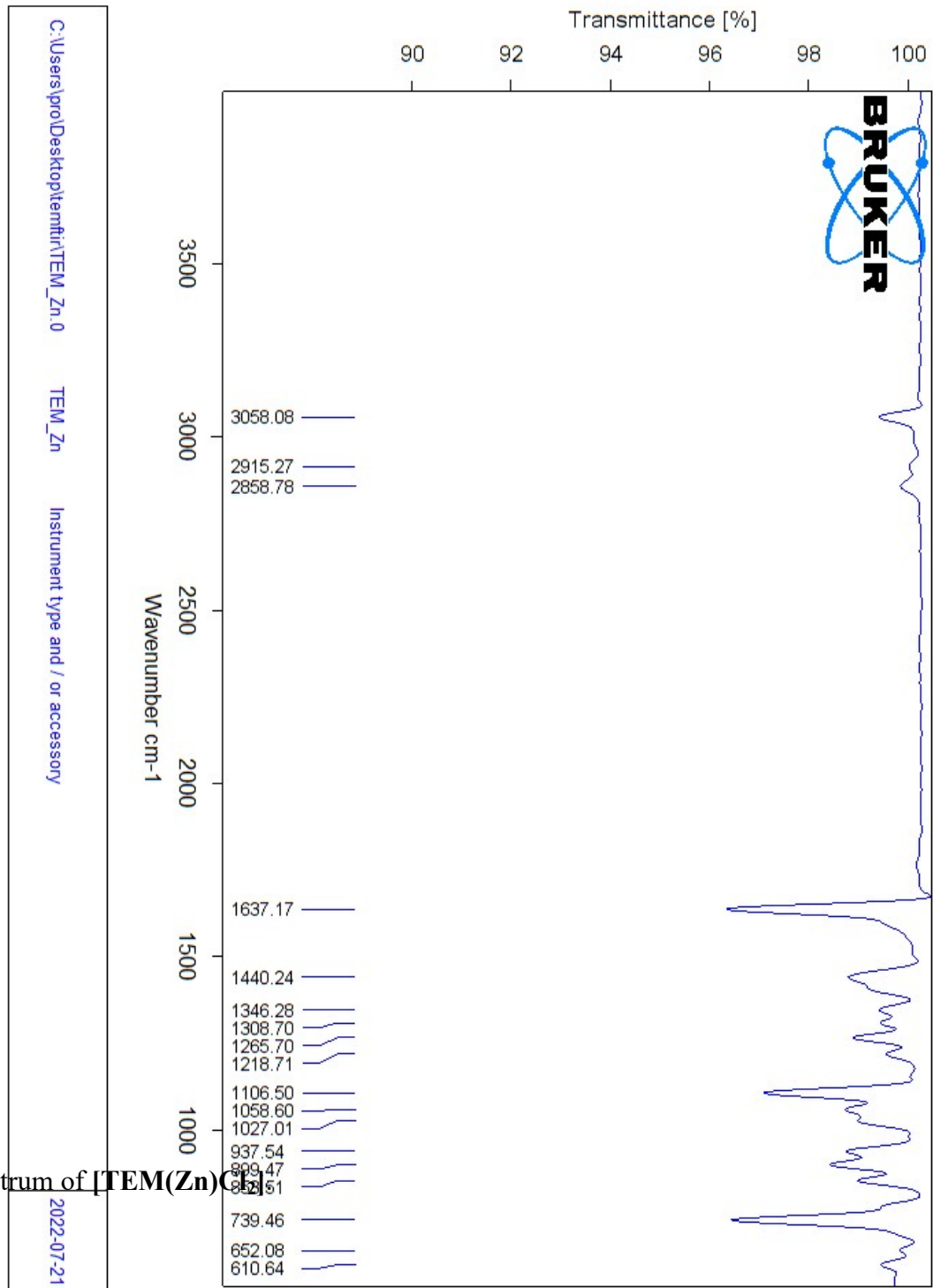


FIGURE S10. FTIR spectrum of [TEM(Zn)Cl]

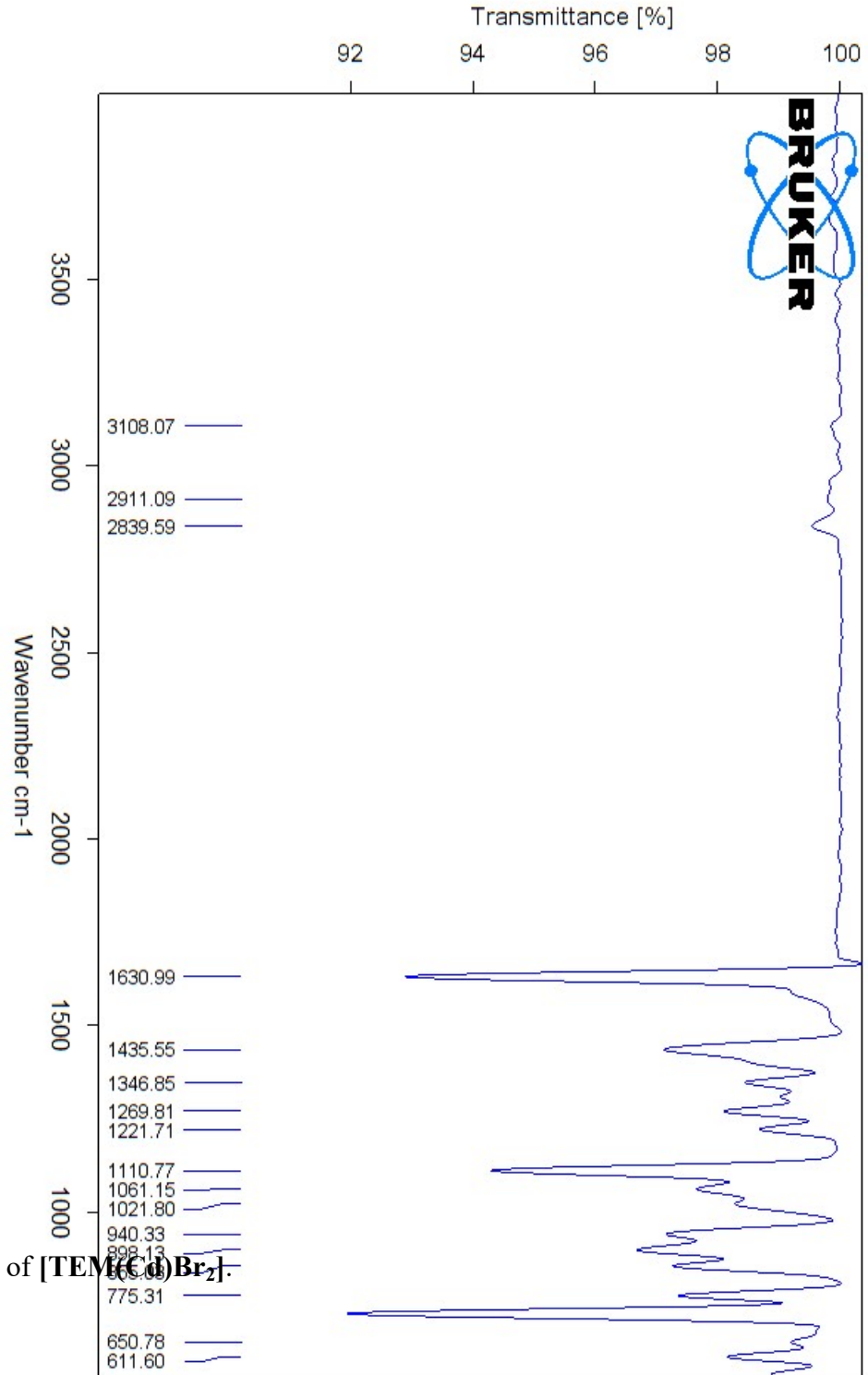


FIGURE S11. FTIR spectrum of [TEM(Cd)Br₂].

EagerSmart Summarize Results

Date : 2022-03-10 at 10:01:48

Method Name : NCHS

Method Filename : EA-C_20220308.mth

Group No : 2	Element %			
Sample Name	Nitrogen	Carbon	Hydrogen	Sulphur
TEM-Cd	6.04276228	26.9035244	3.344803095	0
TEM-Cd	6.038705349	26.88916397	3.335220575	0

2 Sample(s) in Group No : 2

Component Name	Average
Nitrogen	6.040733814
Carbon	26.89634418
Hydrogen	3.340011835
Sulphur	0

Group No : 5	Element %			
Sample Name	Nitrogen	Carbon	Hydrogen	Sulphur
TEM-Zn	7.812420845	36.42247009	4.451468468	0
TEM-Zn	7.8266325	36.56750488	4.446727276	0

2 Sample(s) in Group No : 5

Component Name	Average
Nitrogen	7.819526672
Carbon	36.49498749
Hydrogen	4.449097872
Sulphur	0

Group No : 2	Element %			
Sample Name	Nitrogen	Carbon	Hydrogen	Sulphur
TEM-Cu	8.198022842	36.31325531	4.618414402	0
TEM-Cu	8.262527466	36.41964722	4.642665863	0

2 Sample(s) in Group No : 2

Component Name	Average
Nitrogen	8.230275154
Carbon	36.36645126
Hydrogen	4.630540133
Sulphur	0

Group No : 5	Element %			
Sample Name	Nitrogen%	Carbon%	Hydrogen%	Sulphur%
TEM-Co (EtOH)	7.748516083	36.93906403	4.580291271	0
TEM-Co (EtOH)	7.747725964	36.99332428	4.601635456	0

2 Sample(s) in Group No : 5

Component Name	Average
Nitrogen%	7.748121023
Carbon%	36.96619415
Hydrogen%	4.590963364
Sulphur%	0

FIGURE S12. Summary of elemental analysis of synthesized complexes.

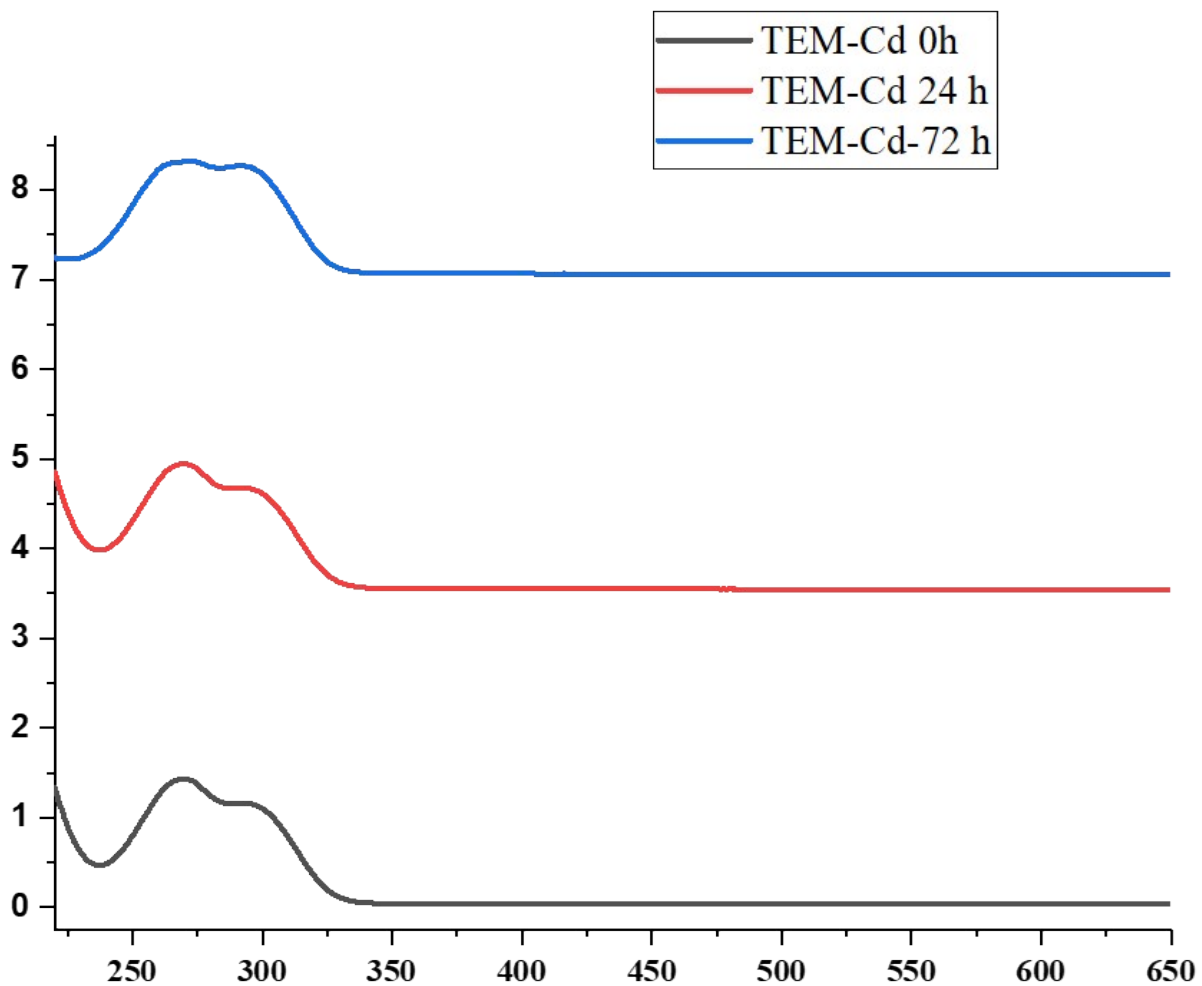


FIGURE S13. Time stability of complex [TEM(Cd)Br₂] followed by UV-Vis spectrophotometry at room temperature in acetonitrile.

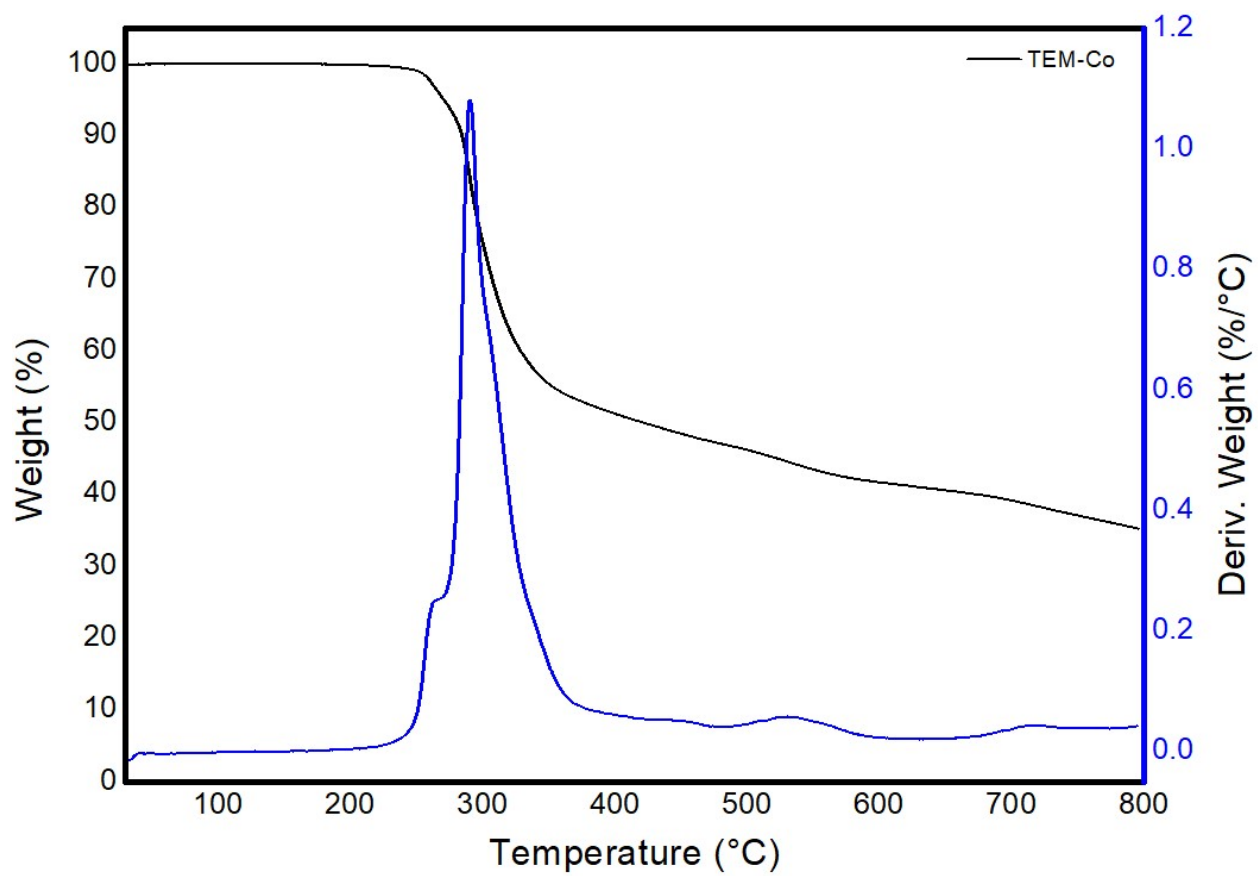


FIGURE S14. TGA thermogram of [TEM(Co)Cl₂].

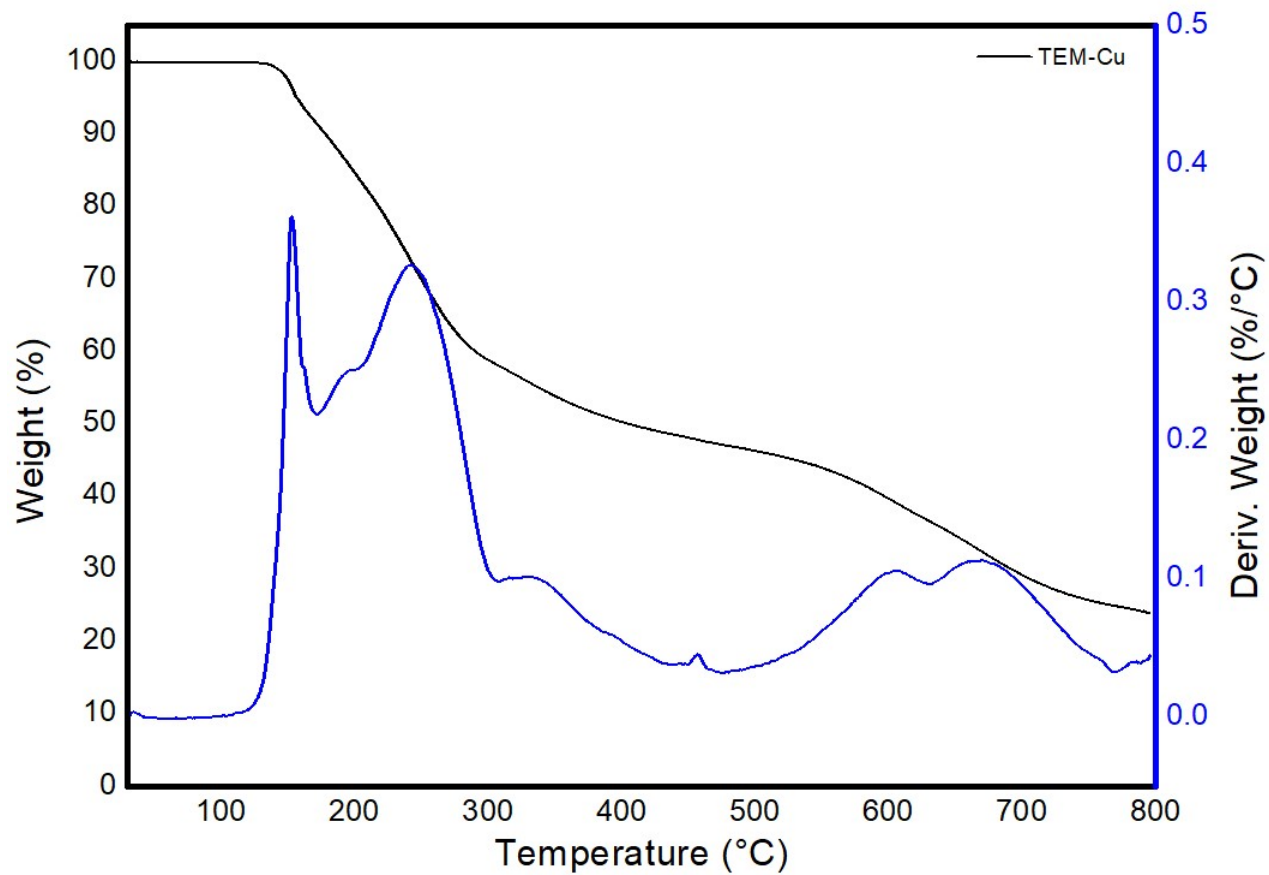


FIGURE S15. TGA thermogram of [TEM(Cu)Cl₂].

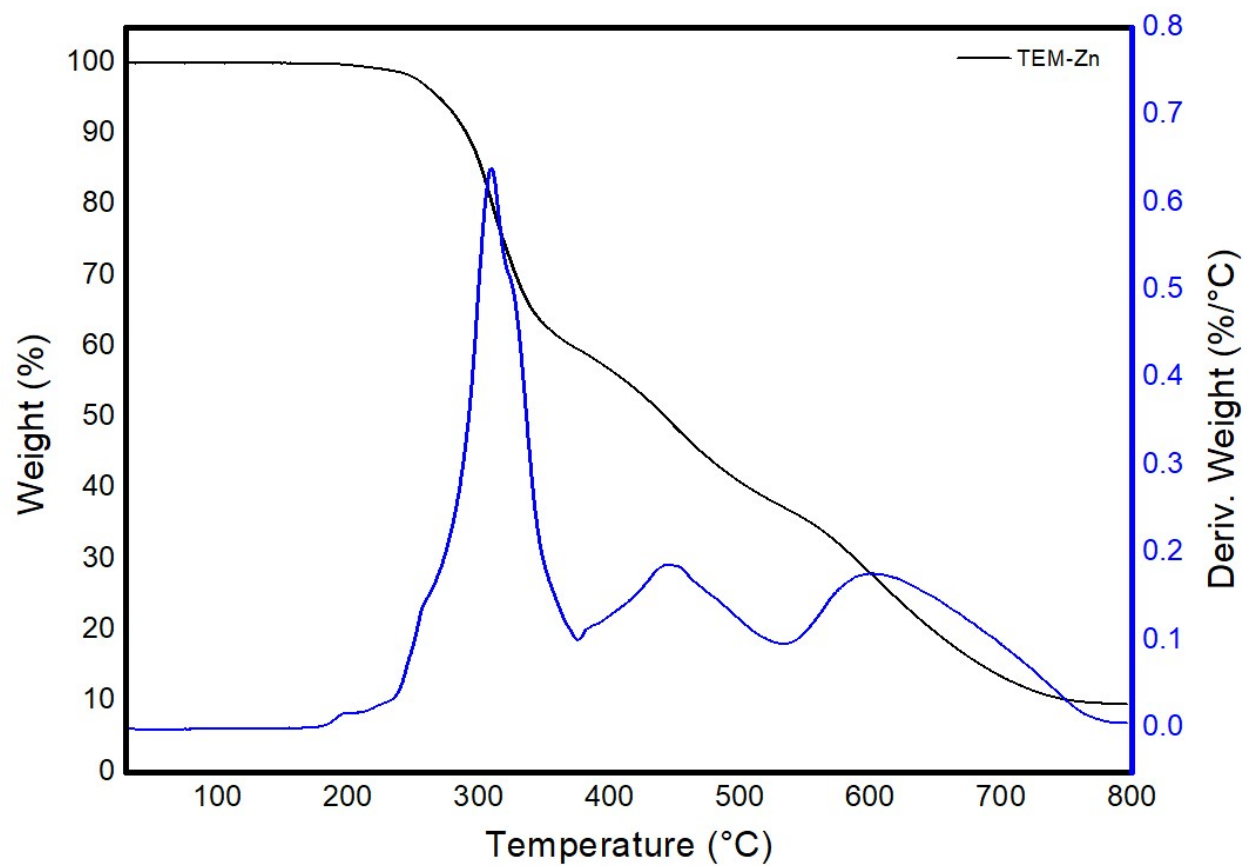


FIGURE S16. TGA thermogram of [TEM(Zn)Cl₂].

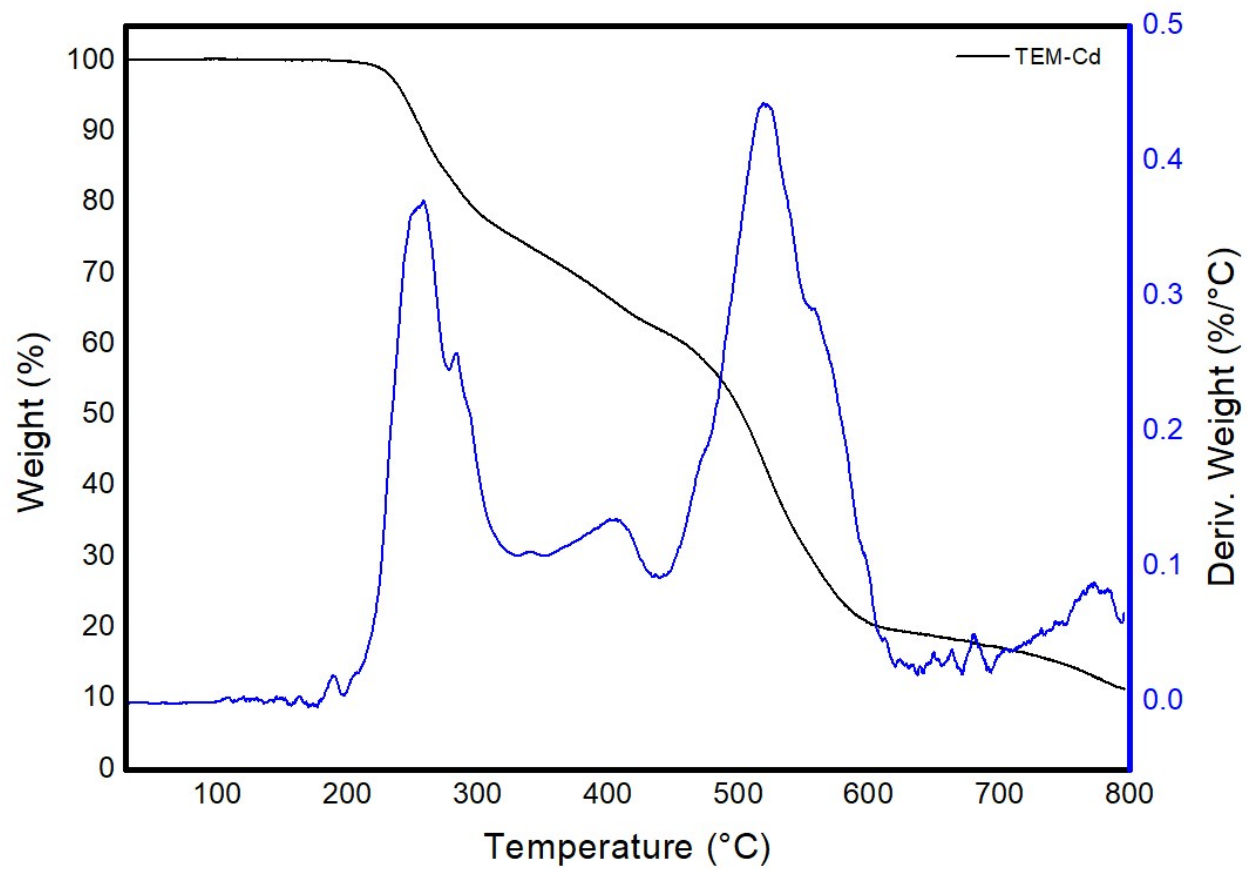
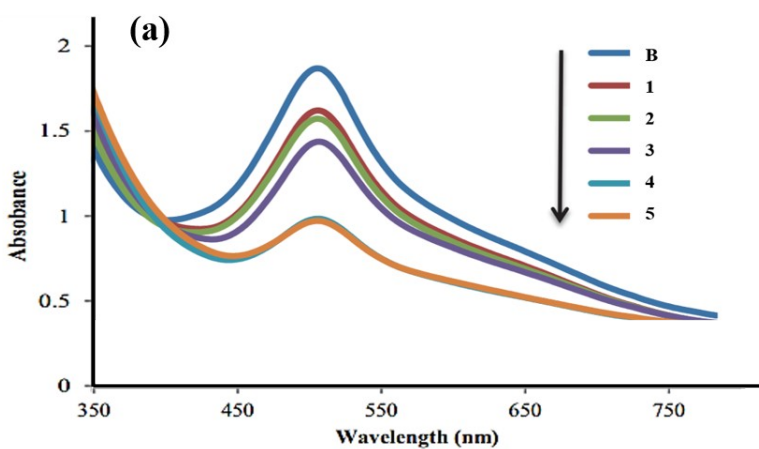


FIGURE S17. TGA thermogram of [TEM(Cd)Br₂].



(b)

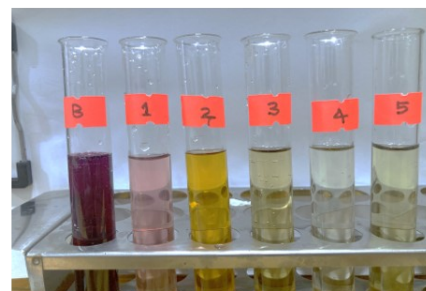


FIGURE S18. (a) Representative absorption spectra of DPPH in the presence and absence of [TEM(Cd)Br₂]. (b) The arrow represents the decrease in absorption with increasing concentration; the change in the solution colour is also shown.

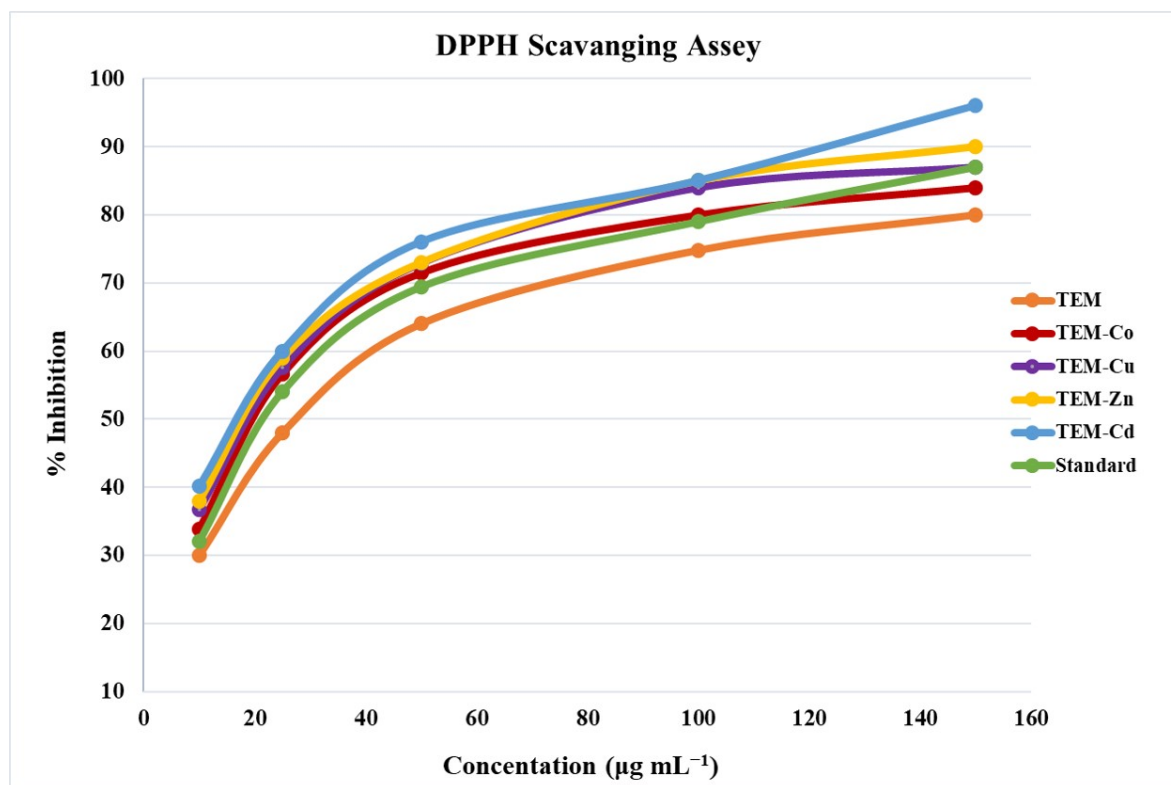


FIGURE S19. Antioxidant activity of TEM and corresponding M(II) complexes.

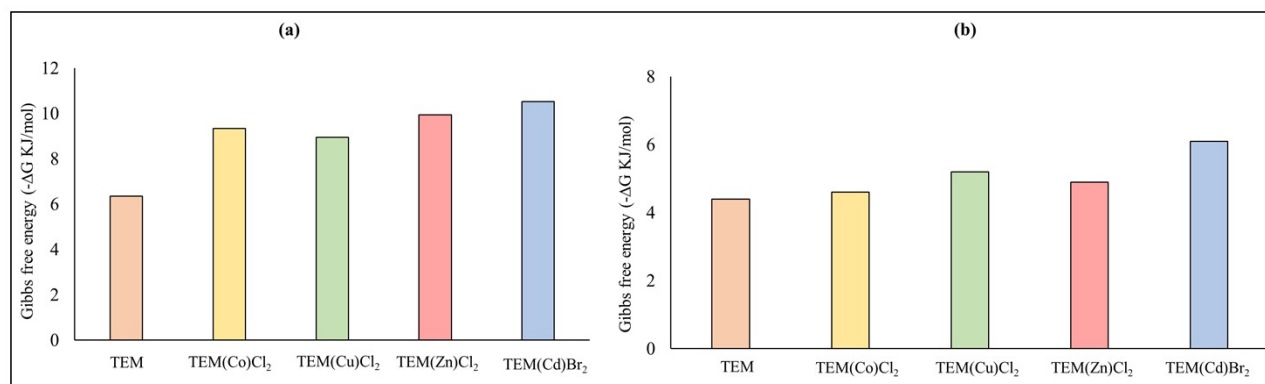


FIGURE S20. Calculated Gibbs free energy of TEM and their metal complexes with **(a)** 2JK6 and **(b)** 2UBP from molecular docking results.

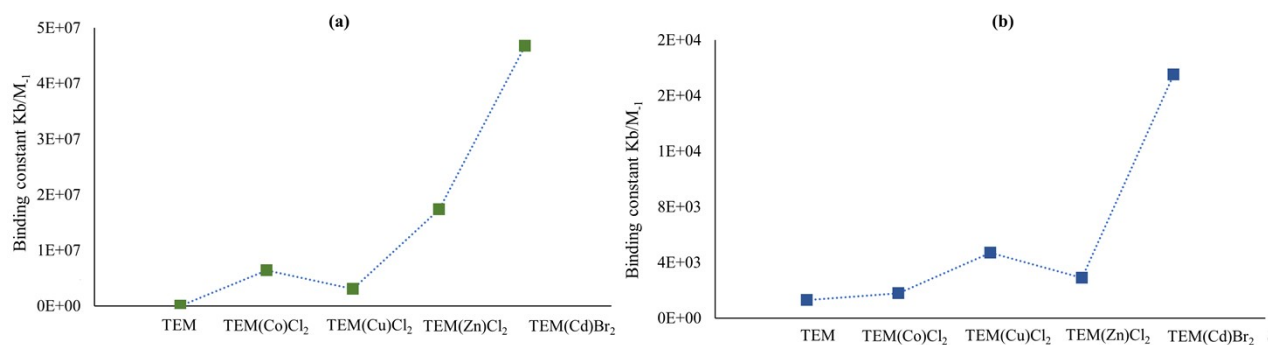


FIGURE S21. Calculated binding constant of **TEM** and their metal complexes with (a) 2JK6 and (b) 2UBP from molecular docking results.

TABLE S1. Structure refinement and crystallographic data of [TEM(M)X₂], (M = Co, Zn; X = Cl; M = Cd, X = Br) complexes.

	[TEM(Co)Cl ₂]	[TEM(Zn)Cl ₂]	[TEM(Cd)Br ₂].CH ₂ Cl ₂
Empirical formula	C ₁₁ H ₁₆ Cl ₂ CoN ₂ OS	C ₁₁ H ₁₆ Cl ₂ N ₂ OSZn	C ₁₁ H ₁₆ Br ₂ CdN ₂ OS. CH ₂ Cl ₂
Formula weight	354.14	360.59	581.46
Temperature (K)	293(2)	293(2)	293(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Monoclinic
Space group	P-1	P-1	P2 ₁ /c
Unit cell dimensions			
<i>a</i> (Å)	8.4030(4)	8.4460(4)	8.6766(3)
<i>b</i> (Å)	9.2421(3)	9.2335(4)	15.4523(6)
<i>c</i> (Å)	9.9135(6)	9.9636(5)	14.4470(4)
<i>α</i> (°)	90.781(4)	90.682(4)	90
<i>β</i> (°)	108.380(5)	108.394(4)°	97.237(3)
<i>γ</i> (°)	90.619(3)	90.304(4)°	90
Volume (Å ³)	730.46(6)	737.24(6)	1921.53(11)

<i>Z</i>	2	2	4
Density (calculated) (Mg/m ³)	1.610	1.624	2.010
Absorption coefficient (mm ⁻¹)	1.659	2.158	5.668
<i>F</i> (000)	362	368	1120
Crystal size (mm ³)	0.143 × 0.121 × 0.089	0.125 × 0.058 × 0.010	0.125 × 0.105 × 0.075
θ range for data collection (°)	2.165 to 30.661	2.154 to 26.366	1.938 to 26.371
Index ranges	-11≤ <i>h</i> ≤11, -13≤ <i>k</i> ≤13, - 13≤ <i>l</i> ≤13	-10≤ <i>h</i> ≤10, -11≤ <i>k</i> ≤11, - 12≤ <i>l</i> ≤12	-10≤ <i>h</i> ≤10, -19≤ <i>k</i> ≤19, - 17≤ <i>l</i> ≤18
Reflections collected	12637	9294	14902
Independent reflections	4212 [R(int) = 0.0440]	2981 [R(int) = 0.0318]	3927 [R(int) = 0.0362]
Completeness to θ = 25.242°	99.4	99.2	100.0
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²	Full-matrix least-squares on <i>F</i> ²
Data/restraints/parameters	4212 / 0 / 163	2987 / 0 / 163	3927 / 0 / 190
Goodness-of-fit on <i>F</i> ²	1.097	1.073	1.122

Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0452, wR_2 = 0.1223$	$R_1 = 0.0356, wR_2 = 0.0873$	$R_1 = 0.0395, wR_2 = 0.0938$
R indices (all data)	$R_1 = 0.0667, wR_2 = 0.1404$	$R_1 = 0.0463, wR_2 = 0.0916$	$R_1 = 0.0549, wR_2 = 0.1064$
Largest diff. peak and hole ($e \cdot \text{\AA}^{-3}$)	0.657 and -0.979	0.442 and -0.549	0.581 and -0.966

TABLE S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for [TEM(Co)Cl₂]. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Co(1)	5047(1)	3420(1)	2592(1)	34(1)
Cl(1)	6096(1)	3099(1)	4921(1)	53(1)
S(1)	8139(1)	5958(1)	3330(1)	66(1)
O(1)	2101(3)	-355(2)	1654(3)	62(1)
N(1)	4137(3)	5413(2)	1945(2)	37(1)
C(1)	4768(3)	6693(3)	2064(3)	40(1)
Cl(2)	6627(1)	2447(1)	1400(1)	58(1)
N(2)	2490(3)	2742(2)	2065(2)	35(1)
C(2)	6502(3)	7115(3)	2648(3)	43(1)
C(3)	7084(4)	8543(3)	2773(3)	52(1)
C(4)	8781(5)	8661(4)	3393(4)	73(1)
C(5)	9526(4)	7360(5)	3750(4)	74(1)
C(6)	2293(3)	5297(3)	1331(3)	45(1)
C(7)	1670(3)	4146(3)	2124(3)	42(1)
C(8)	1758(4)	2043(3)	635(3)	45(1)
C(9)	2435(4)	533(3)	606(3)	55(1)
C(10)	2125(4)	1760(3)	3114(3)	45(1)
C(11)	2825(4)	288(3)	3026(4)	57(1)

TABLE S3. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for [TEM(Zn)Cl₂]. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Zn(1)	4941(1)	6611(1)	7403(1)	34(1)
Cl(1)	3928(1)	6911(1)	5086(1)	51(1)
S(1)	1842(1)	4057(1)	6640(1)	64(1)
O(1)	7915(4)	10355(3)	8347(3)	62(1)
N(1)	5834(3)	4577(3)	8045(3)	36(1)
C(1)	5204(4)	3306(3)	7916(3)	38(1)
Cl(2)	3409(1)	7559(1)	8628(1)	56(1)
N(2)	7523(3)	7253(3)	7948(3)	34(1)
C(2)	3480(4)	2896(4)	7335(3)	41(1)
C(3)	2906(5)	1467(4)	7214(4)	47(1)
C(4)	1175(6)	1362(5)	6589(5)	68(1)
C(5)	452(5)	2656(5)	6231(5)	73(1)
C(6)	7673(4)	4690(4)	8664(4)	44(1)
C(7)	8299(4)	5830(3)	7884(4)	42(1)
C(8)	8255(4)	7949(4)	9368(3)	44(1)
C(9)	7589(5)	9465(4)	9402(4)	54(1)
C(10)	7206(5)	9715(4)	6993(4)	55(1)
C(11)	7889(4)	8228(4)	6904(4)	44(1)

TABLE S4. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $[\text{TEM}(\text{Cd})\text{Br}_2] \cdot \text{CH}_2\text{Cl}_2$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cd(1)	3909(1)	6906(1)	6223(1)	38(1)
Br(1)	1390(1)	7368(1)	6788(1)	51(1)
Cl(1)	-742(1)	4643(1)	8074(1)	65(1)
S(1)	2622(2)	4834(1)	6302(1)	60(1)
O(1)	6428(4)	9303(2)	6298(2)	61(1)
N(1)	4536(3)	8018(2)	5235(2)	34(1)
C(1)	2902(4)	5503(3)	4527(3)	45(1)
Br(2)	6150(1)	6364(1)	7340(1)	63(1)
Cl(2)	-281(2)	6134(1)	9292(1)	89(1)
N(2)	3543(4)	6215(2)	4807(2)	40(1)
C(2)	2338(5)	4844(3)	5103(3)	46(1)
C(3)	1465(5)	4142(3)	4760(3)	52(1)
C(4)	1042(5)	3618(3)	5476(4)	59(1)
C(5)	1581(6)	3903(3)	6332(3)	62(1)
C(6)	4039(5)	6809(3)	4100(3)	48(1)
C(7)	3701(5)	7735(3)	4324(2)	43(1)
C(8)	3929(5)	8871(2)	5492(3)	44(1)
C(9)	4814(5)	9208(3)	6379(3)	58(1)
C(10)	7038(5)	8494(3)	6068(3)	58(1)
C(11)	6223(4)	8130(3)	5176(3)	50(1)
C(12)	202(6)	5628(3)	8307(4)	73(1)