Molecules

Synthesis, structural characterization and electrochemical properties of Copper(II) complexes with Functionalized Thiosemicarbazones derived from 5-Acetylbarbituric Acid

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Supplementary material

Table S1. Hydrogen bond parameters [Å, º] for [Cu(HAcbDM)(H_2O)$_2$](NO_3)·H_2O (**3a**), [Cu(HAcbDM)(H_2O)$_2$]ClO_4 (**4**), [Cu(HAcbHexim)Cl] (**6**). The letters in brackets refer to the symmetry codes shown in the text and figures.

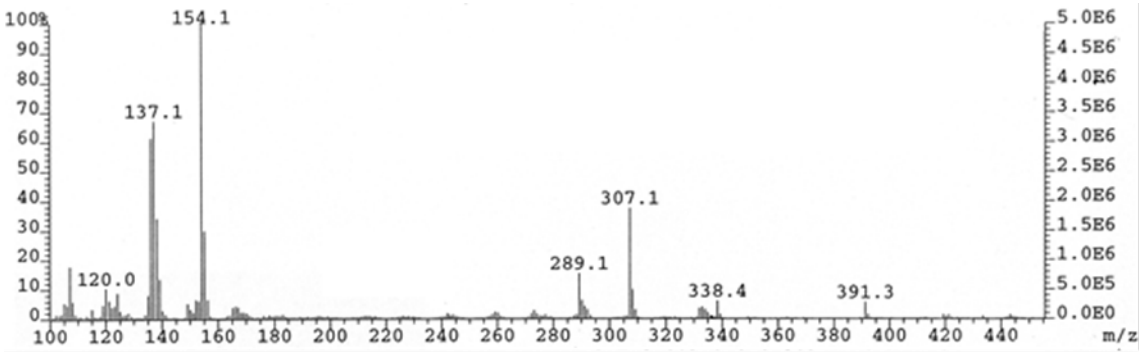
Compound	D–H···A	D–H	H···A	D···A	∠DHA	Symmetry code
3a	O(12)-H(12A)···O(31)[a]	0.94	1.83	2.753(6)	169.5	-x+1,-y+1,-z+1
	O(12)-H(12B)···O(14)[b]	0.92	1.86	2.743(5)	160.3	-x+2,-y+1,-z+1
	O(14)-H(14A)···O(1)	0.95	2.24	2.902(6)	126.1	
	O(14)-H(14B)···O(23)[d]	0.87	1.91	2.775(5)	169.8	-x+1,-y,-z+1
	N(11)-H(11)···O(23)[e]	0.93	1.88	2.789(5)	167.0	x+1,y+1,z
	N(13)-H(13)···O(42)	0.90	2.29	3.084(7)	147.4	
	N(15)-H(15)···O(15)[f]	0.89	1.95	2.829(5	170.9	-x+2,-y+1,-z
	O(22)-H(22B)···O(41)[g]	0.95	1.70	2.646(5)	176.8	-x+1,-y,-z
	O(24)-H(24A)···O(2)	0.93	2.09	2.765(6)	128.0	
	O(24)-H(24B)···O(22)[h]	0.91	1.86	2.699(5)	152.2	-x,-y,-z
	N(21)-H(21)···O(13)[i]	0.94	1.88	2.784(5	159.2	x-1,y-1,z
	N(23)-H(23)···O(32)	1.06	2.16	3.165(8)	157.0	
	N(25)-H(25)···O(1)[d]	0.97	1.90	2.865(5)	171.4	-x+1,-y,-z+1
	O(1)-H(1A)···O(43)	1.05	1.91	2.879(7)	152.1	
	O(1)-H(1B)···O(25)[c]	1.04	1.77	2.802(6)	169.5	x+1,y,z
	O(2)-H(2B)···O(32)	0.90	2.54	3.411(9)	163.9	
4	O(1)-H(1A)···O(2)[a]	0.96	1.83	2.680(12)	146.1	-x+1,-y,-z+1
	O(1)-H(1B)···O(16)[b]	0.96	2.09	2.716(12)	121.7	-x+1/2,y-1/2,-z+1/2
	O(2)-H(2A)···O(13)[c]	0.96	2.01	2.856(11)	146.6	x,y,z-1
	O(2)-H(2B)···O(18A)	0.96	2.61	3.24(2)	123.5	
	O(2)-H(2B)···O(18B)	0.96	2.21	3.11(3)	156.2	
	N(11)-H(11)···O(13)[d]	0.86	2.06	2.915(13)	175.7	-x+1,-y,-z+2
	N(15)-H(15)···O(18A)[e]	0.86	2.29	3.14(2)	172.8	x,y,z+1
	N(15)-H(15)···O(19B)[e]	0.86	2.28	3.06(3)	150.4	x,y,z+1
6	N(11)-H(11A)···O(15)[a]	0.84(3)	2.04(3)	2.851(3)	162(3)	-x+1,y-1/2,-z+1/2
	N(13)-H(13A)···O(13)[b]	0.86(3)	2.19(3)	2.939(3)	145(3)	x-1/2,y,-z+1/2
	N(15)-H(15A)···Cl(1)[c]	0.80(3)	2.72(3)	3.437(2)	151(3)	-x+1,y+1/2,-z+1/2

Table S2. Intermolecular ring-ring and ring-metal interaction parameters (Å, º) for $[Cu(HAcbDM)(H_2O)_2]ClO_4$ (**4**)*.

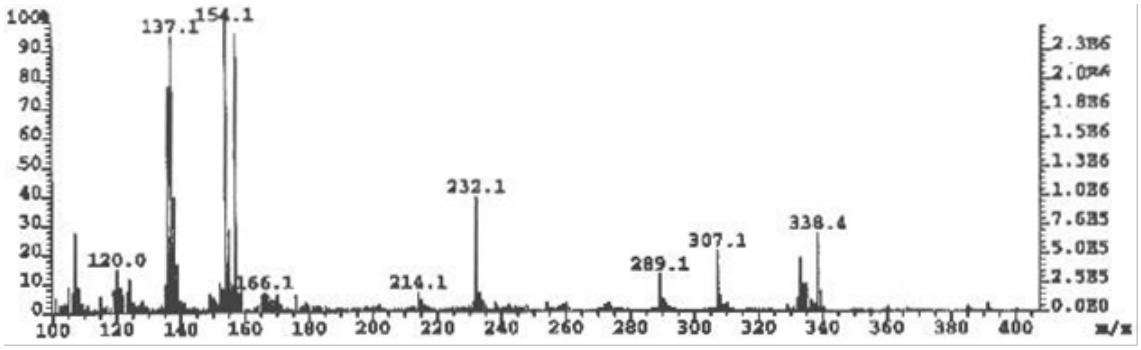
Ring	π···π	Cg-Cg	α	IPD	Symmetry
Cu1/S1/C18/N13/N12	Cg1-Cg1[a]	3.7151	0	3.6077	-x,-y,1-z
Cu1/S1/C18/N13/N12 Cu1/O11/C11/C16/C17/N12	Cg1-Cg2[a]	3.8532	5	3.6203	-x,-y,1-z
Cu1/O11/C11/C16/C17/N12 Cu1/S1/C18/N13/N12	Cg2-Cg1[a]	3.8532	5	3.4833	-x,-y,1-z
Cu1/S1/C18/N13/N12	Cg1-Cu1[a]	3.911	22.51		-x,-y,1-z

*CgI/CgJ are the centroids of the corresponding rings. Cg-Cg is the center-to-center distance (distance between ring centroids), α is the angle between mean planes of the rings, IPD is the mean interplanar distance (distance from one plane to the neighboring centroid). For details, see Janiak, C. (2000). J. Chem. Soc. Dalton Trans. pp. 3885–3898.

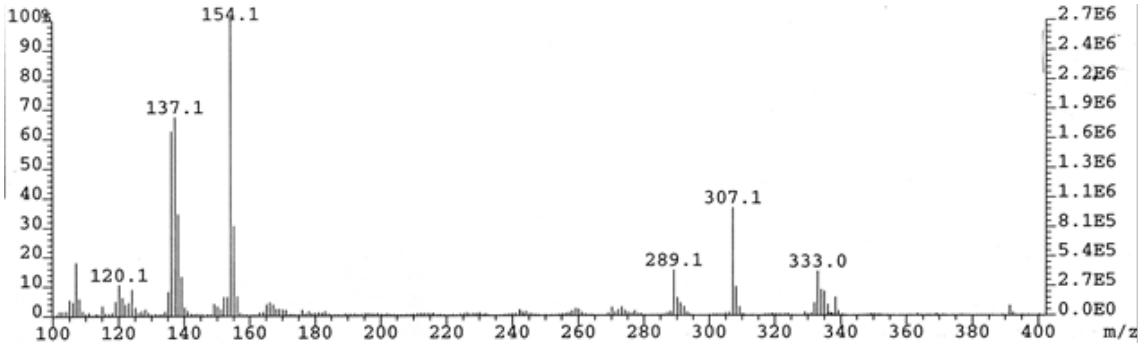
Figure S1. Mass spectra of the complexes (FAB).



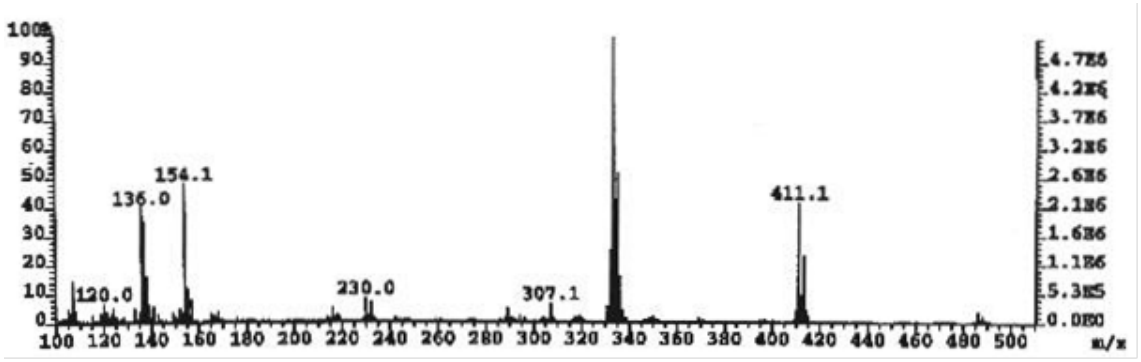
[Cu(HAcbDM)(OAc)]·3H₂O (**1**·3H₂O)



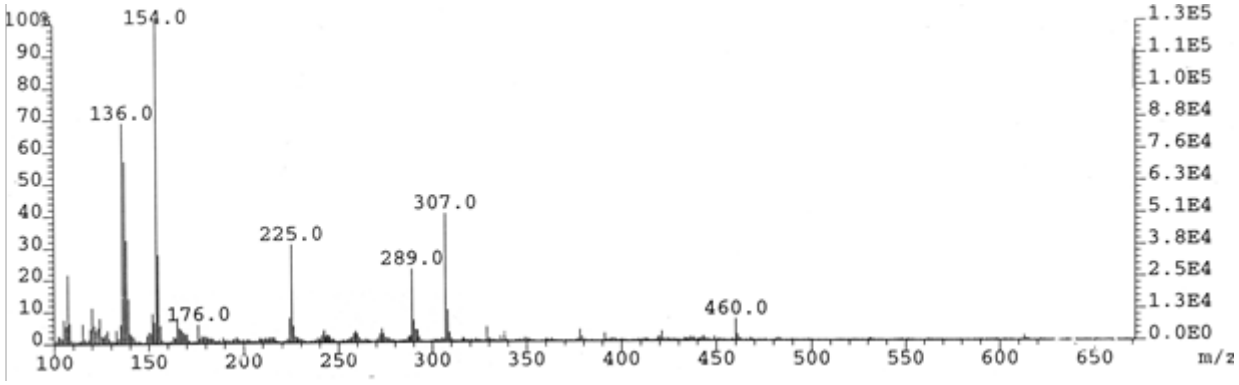
[Cu(HAcbDM)Cl]·1/2EtOH (**2**·1/2EtOH)



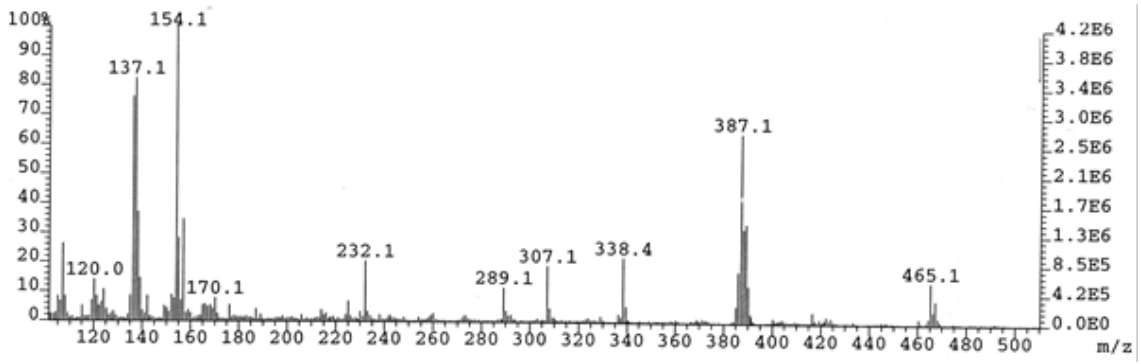
[Cu(HAcbDM)(NO₃)] (**3**)



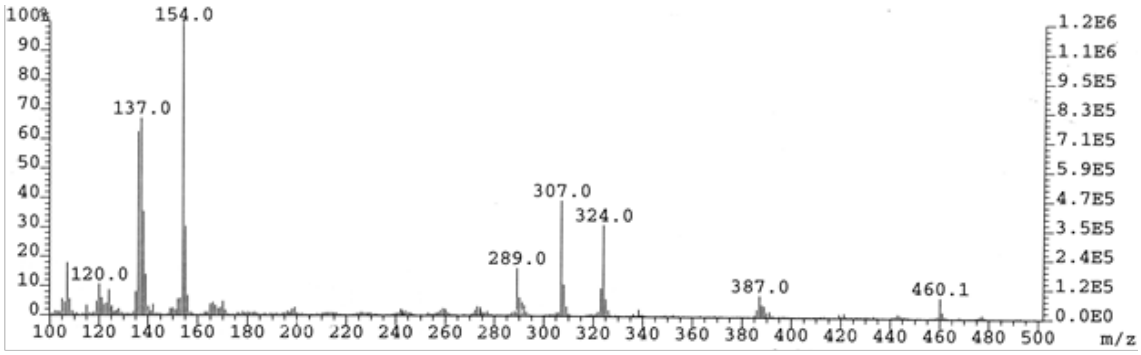
[Cu(HAcbDM)(H₂O)₂]ClO₄ (**4**)



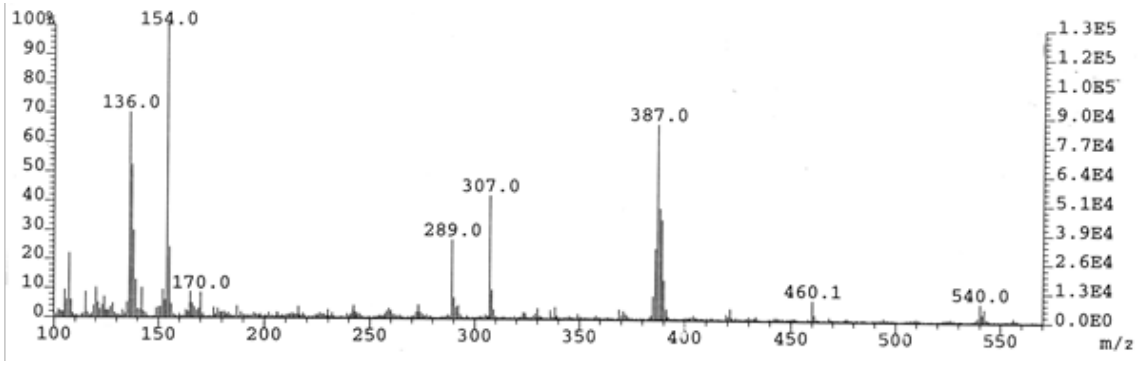
[Cu(HAcbHexim)(OAc)]·5H₂O (**5**·5H₂O)



[Cu(HAcbHexim)Cl]·1/2EtOH (**6**·1/2EtOH)

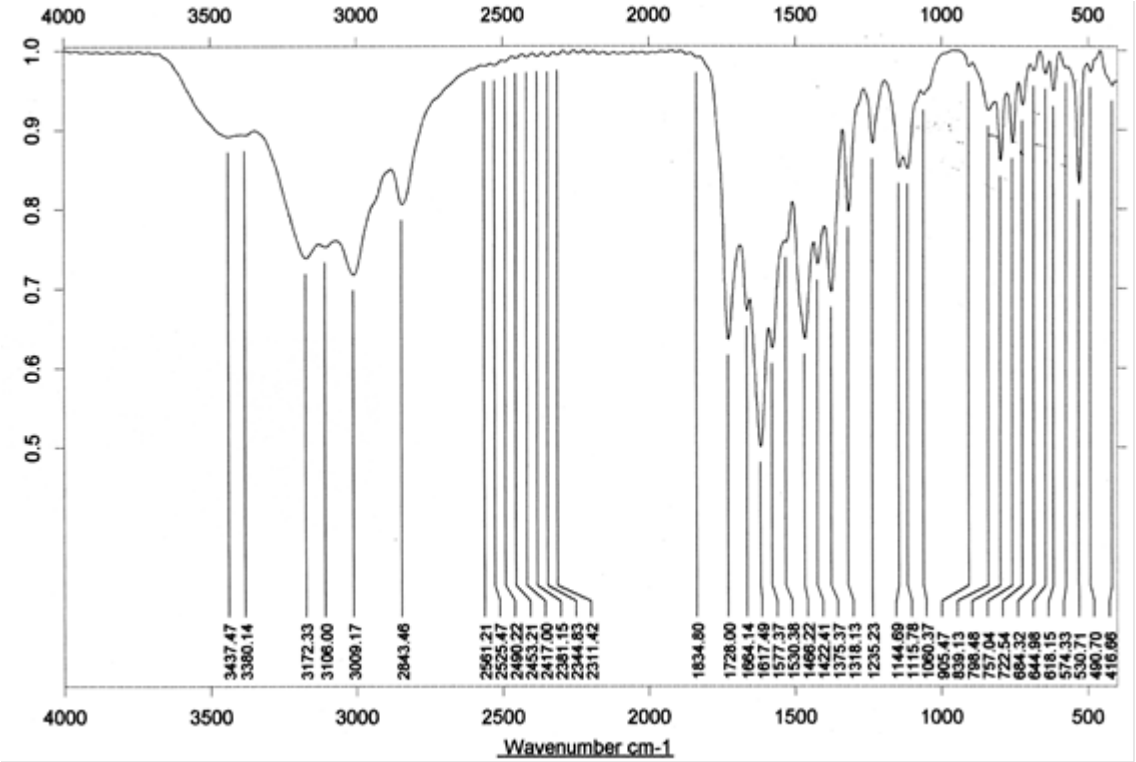


[Cu(HAcbHexim)(NO₃)]·1/2H₂O (**7**·1/2H₂O)

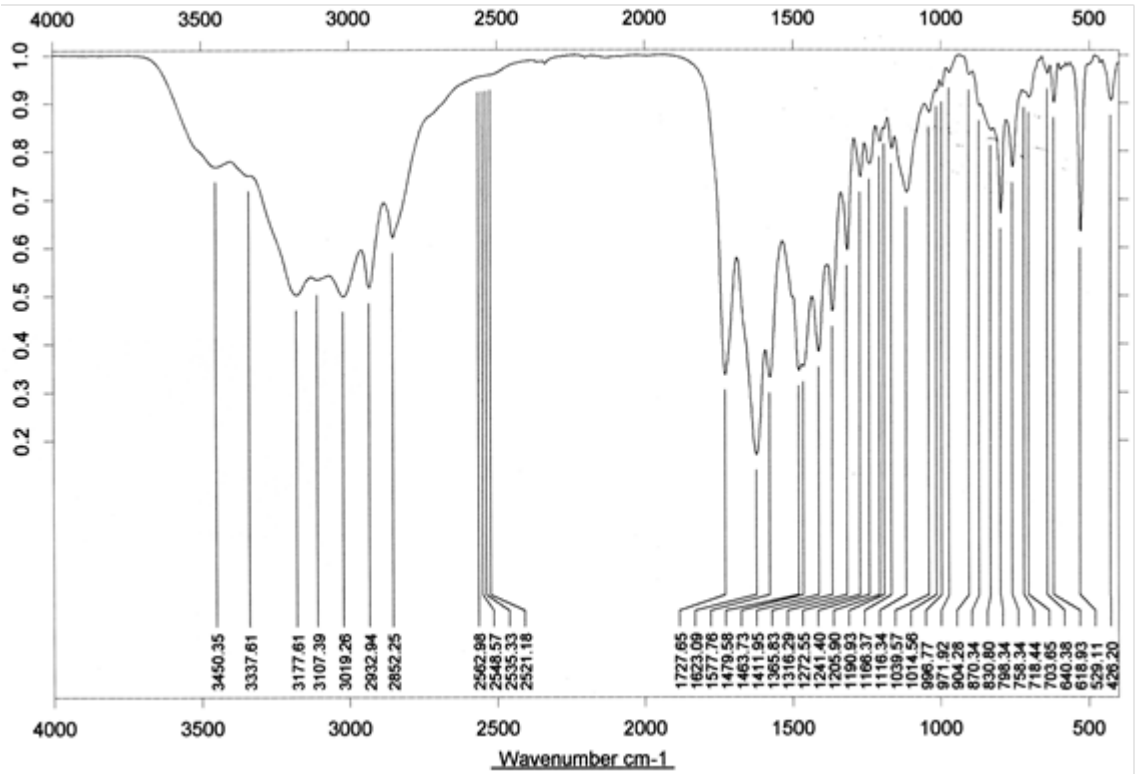


[Cu(HAcbHexim)ClO₄] (**8**)

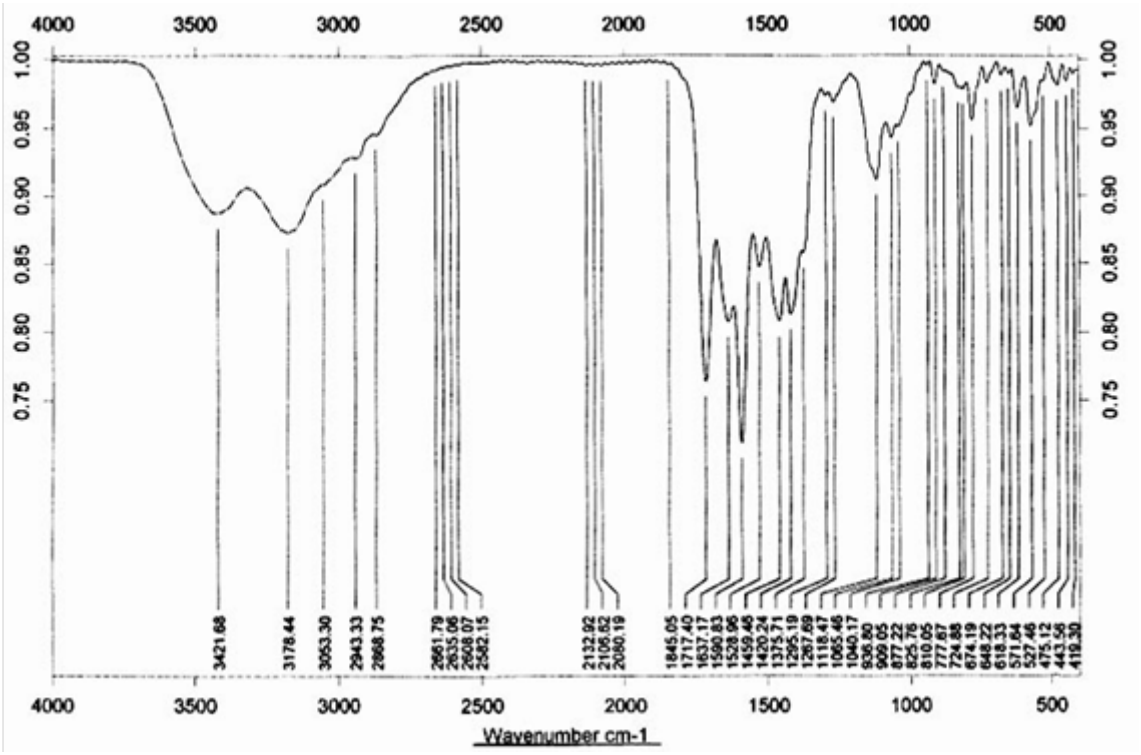
Figure S2. FT-IR spectra in the region 4000-500 cm^{-1}



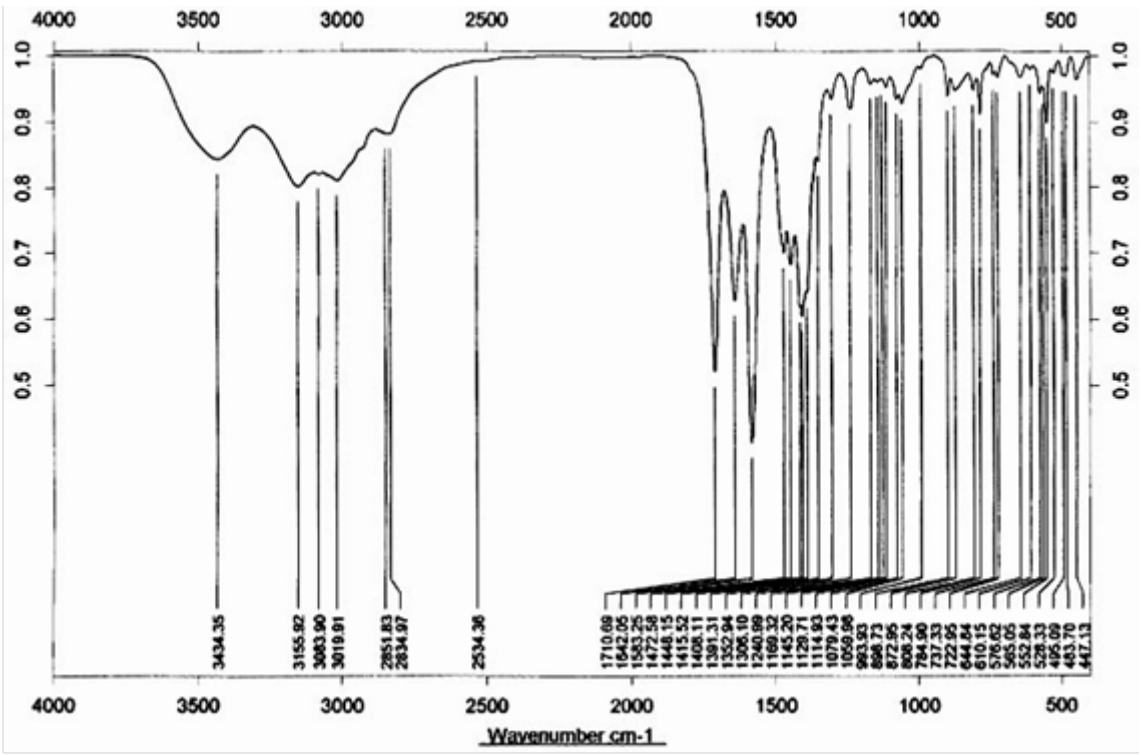
H_2AcbDM·H_2O



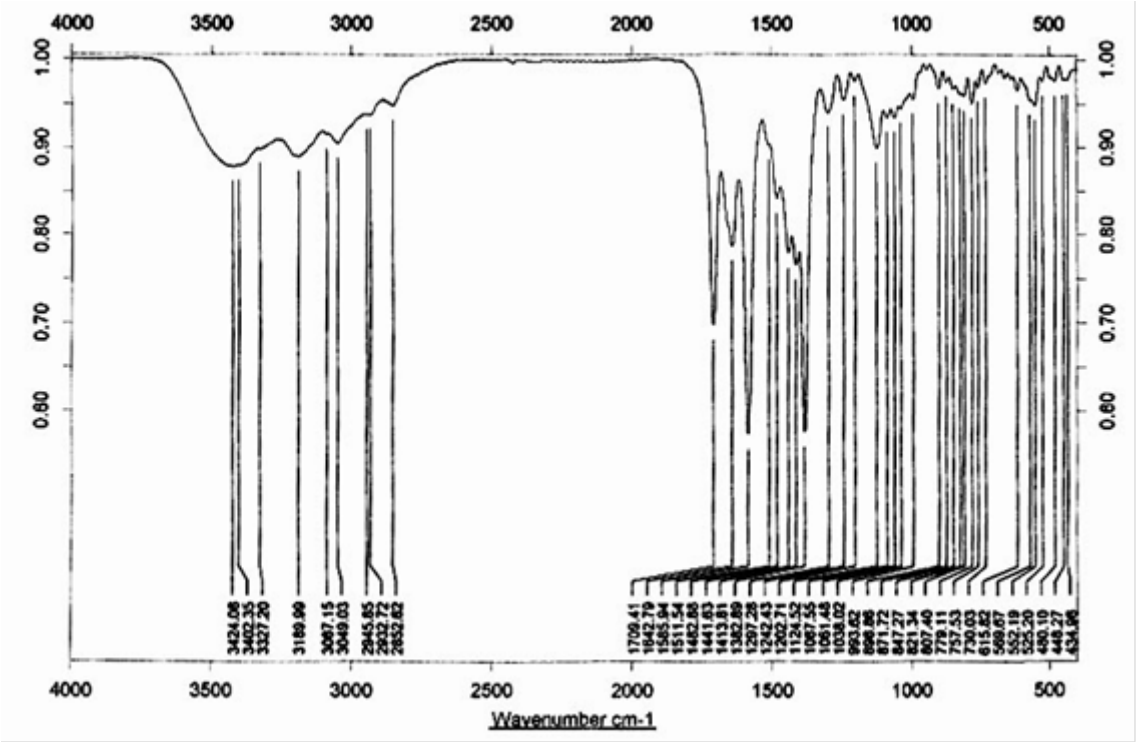
H_2AcbHexim·H_2O



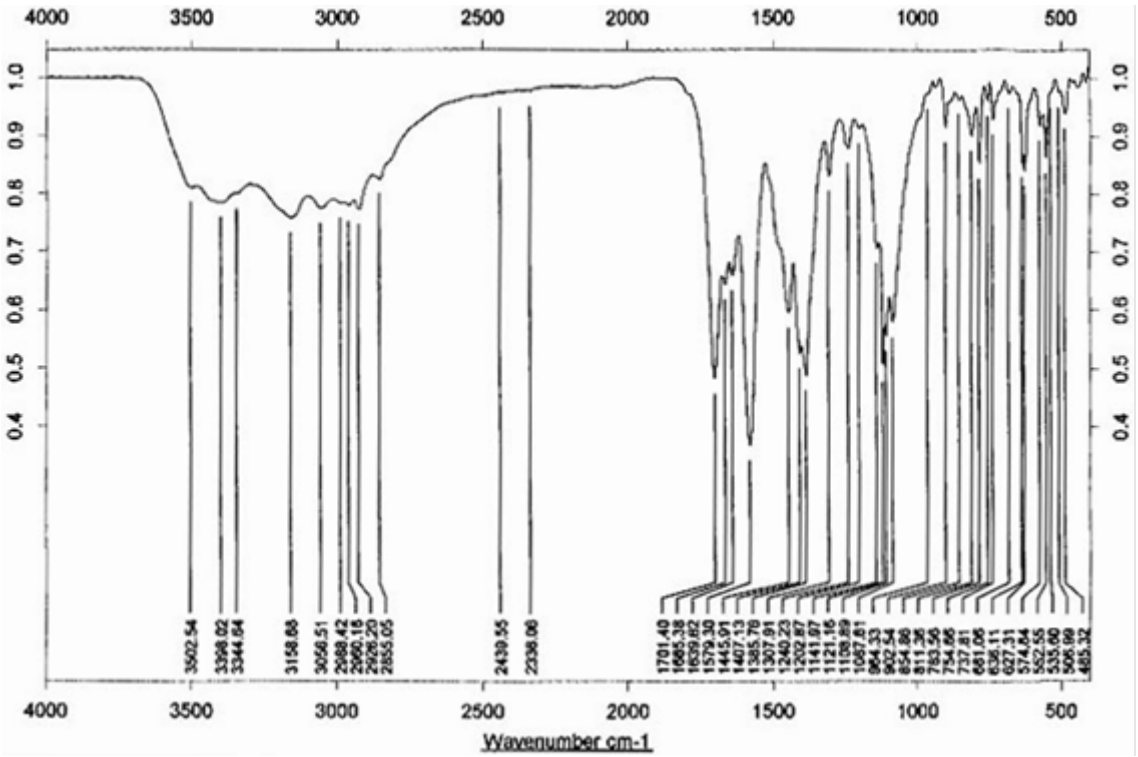
[Cu(HAcbDM)(OAc)]·3H₂O



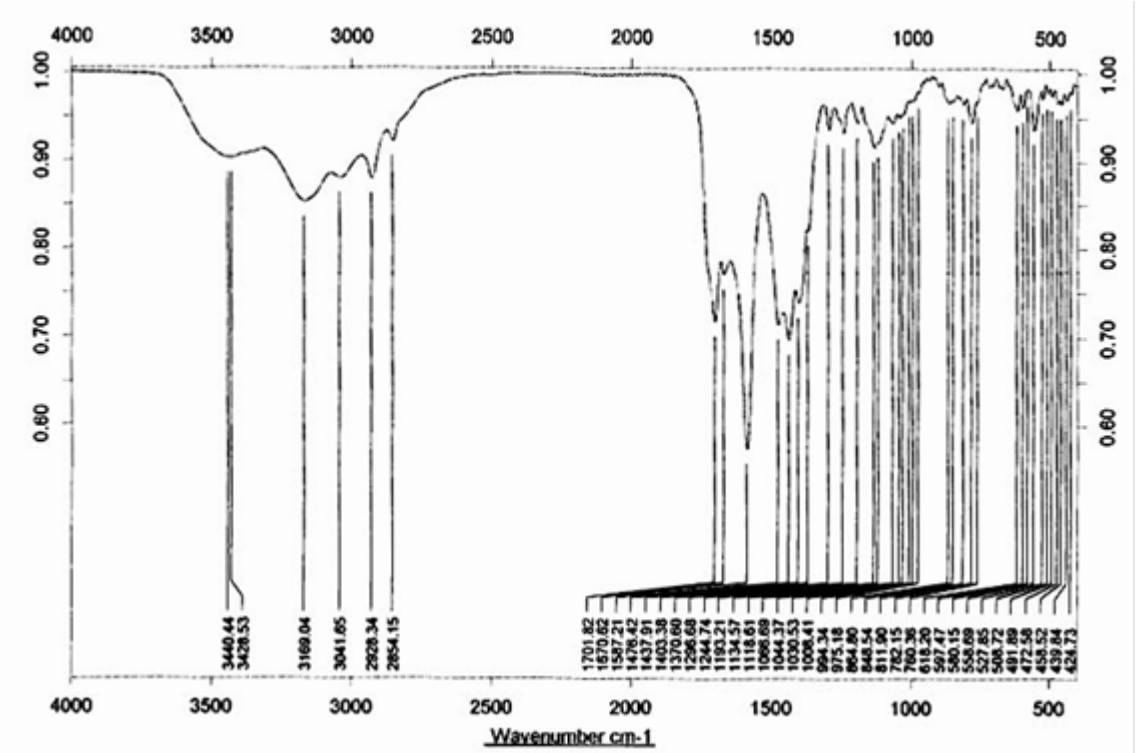
[Cu(HAcbDM)Cl]·1/2EtOH



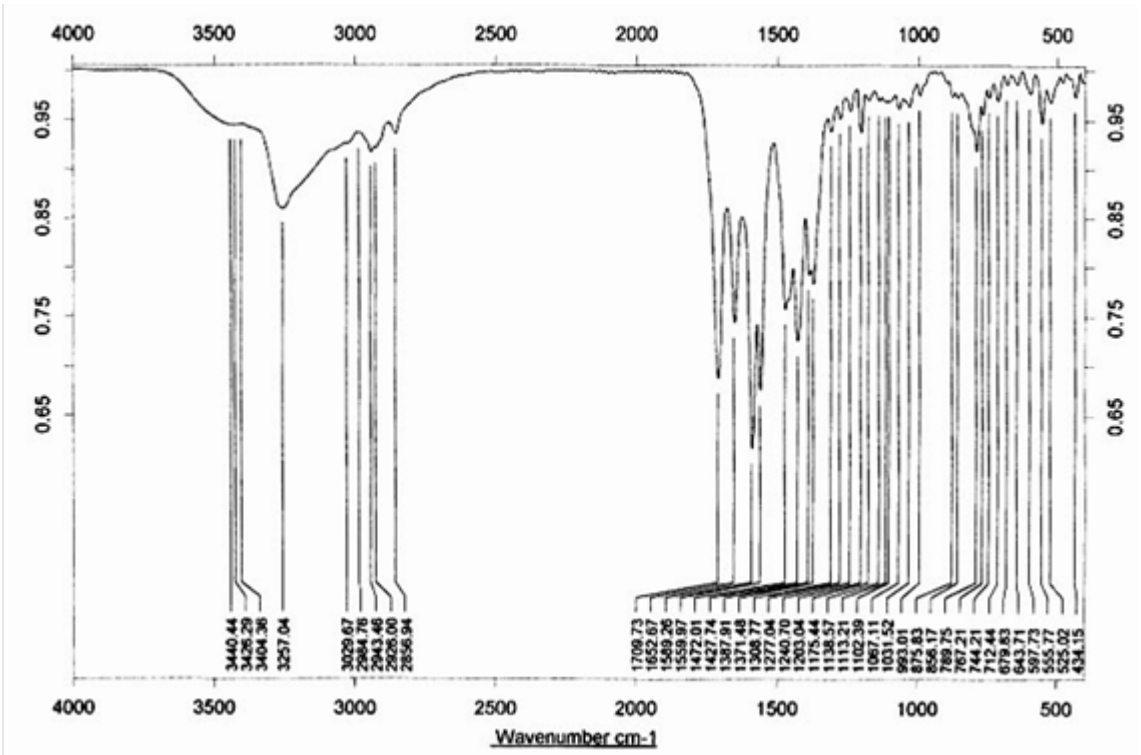
[Cu(HAcbDM)(NO₃)]



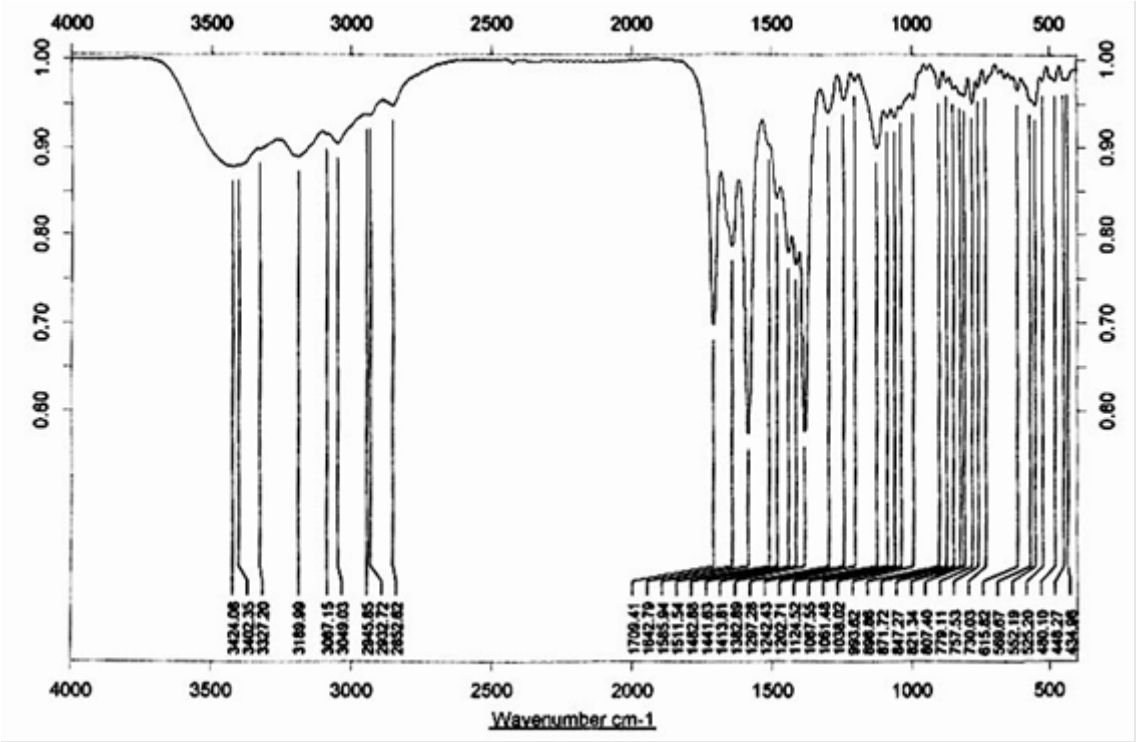
[Cu(HAcbDM)(H₂O)₂]ClO₄



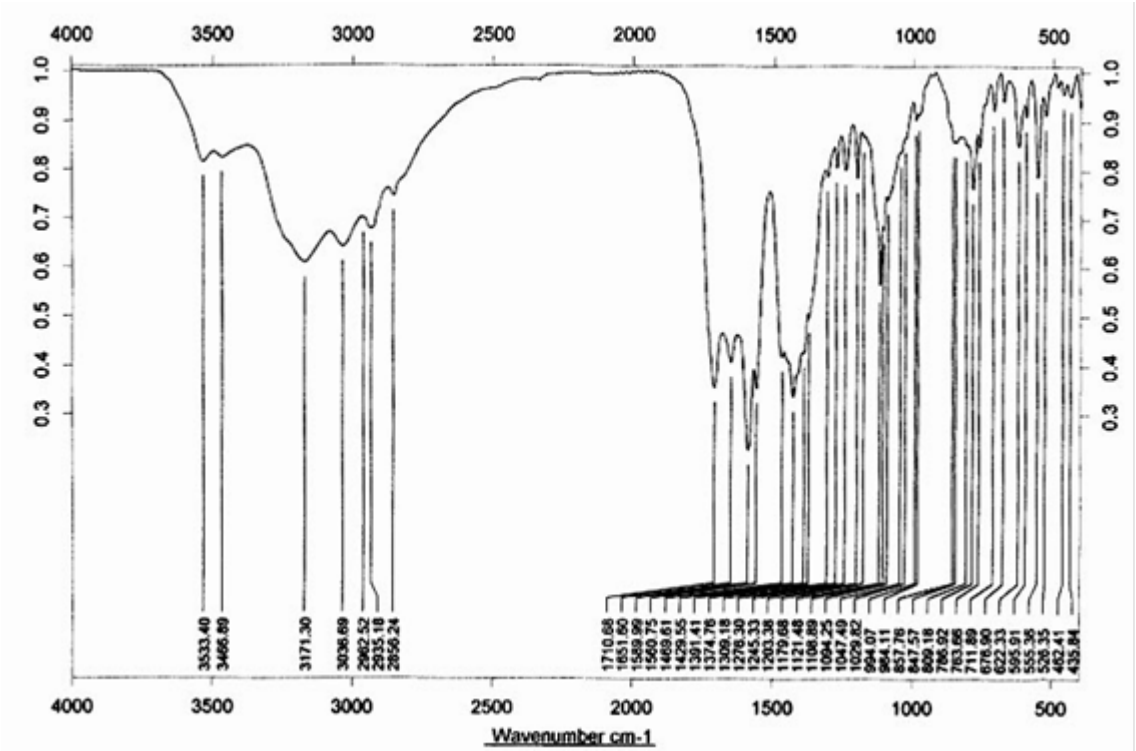
[Cu(HAcbHexim)(OAc)]·5H₂O



[Cu(HAcbHexim)Cl]·1/2EtOH

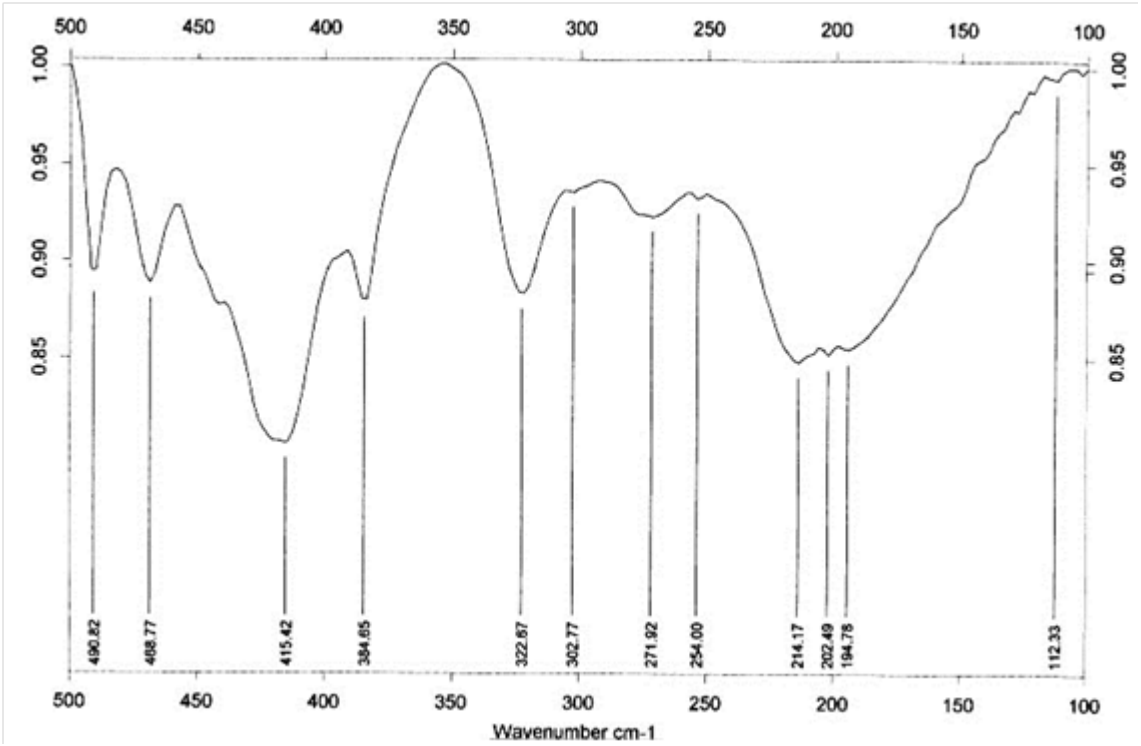


[Cu(HAcbHexim)(NO₃)]·1/2H₂O

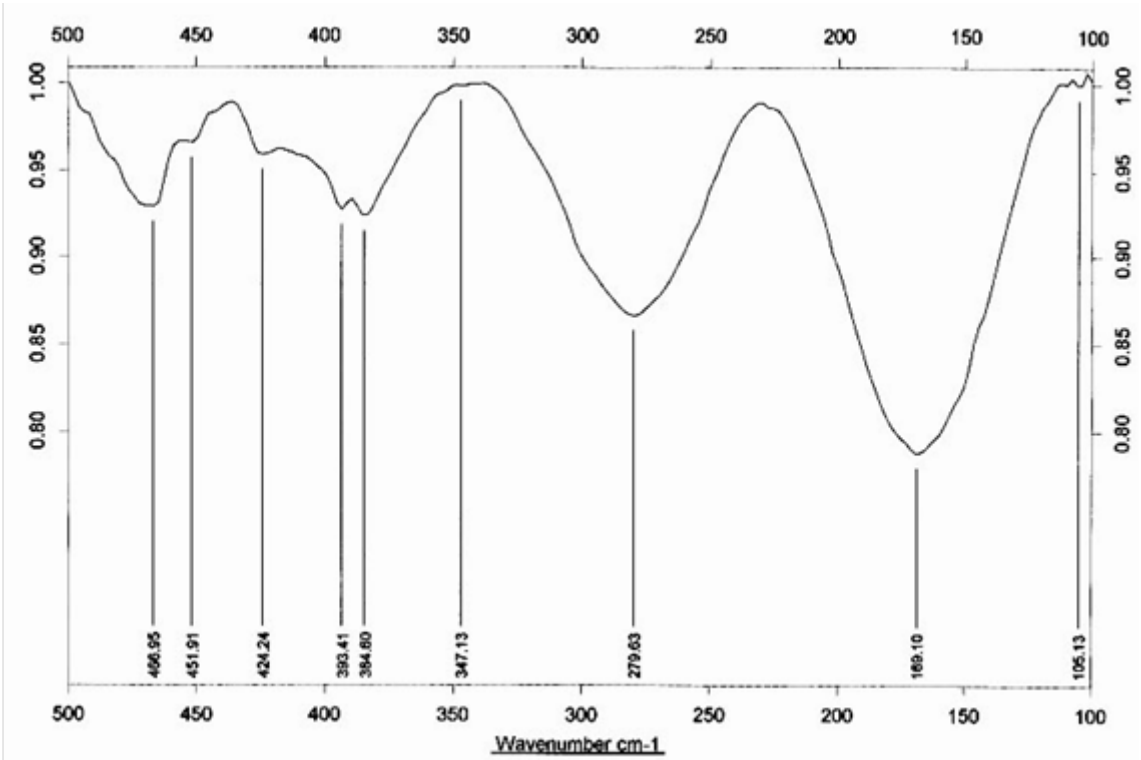


[Cu(HAcbHexim)ClO₄]

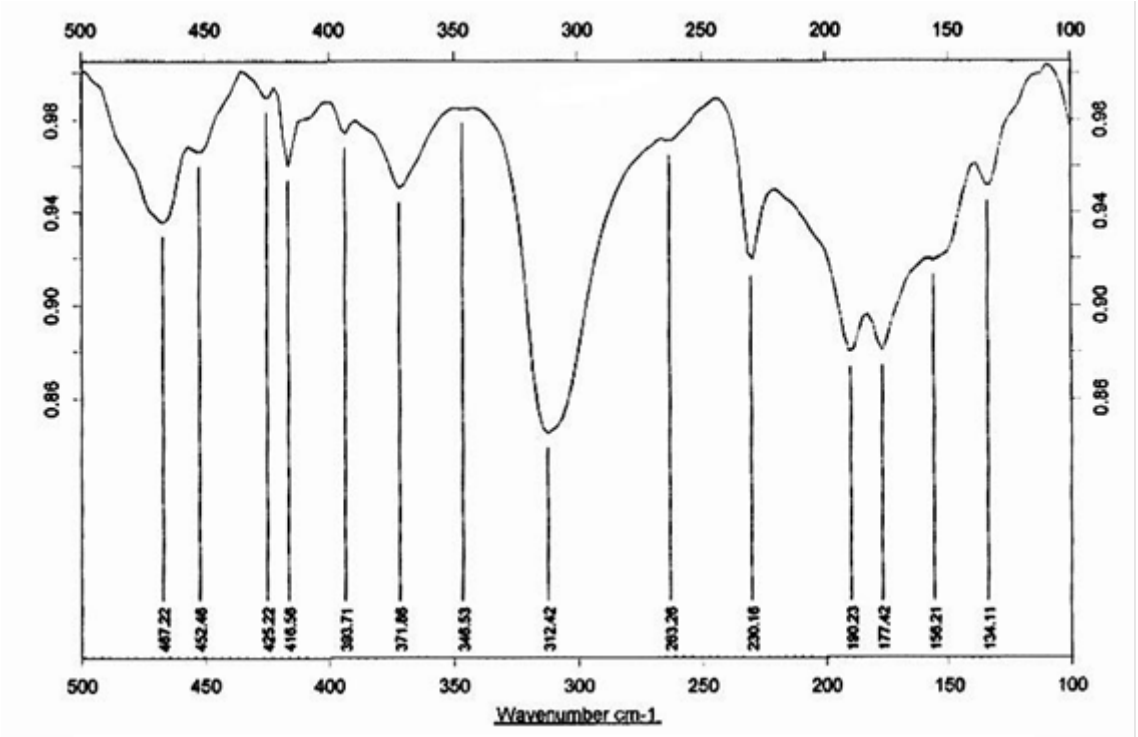
Figure S3. FT-IR spectra in the region 500-100 cm^{-1}



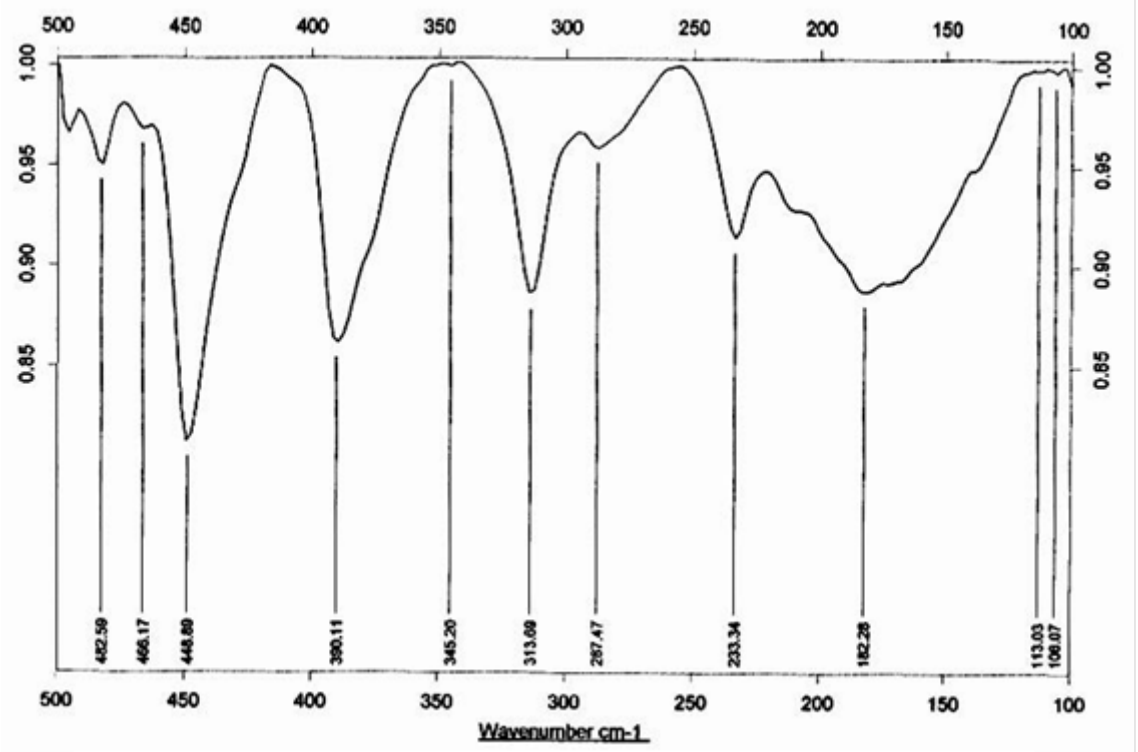
H_2AcbDM·H_2O



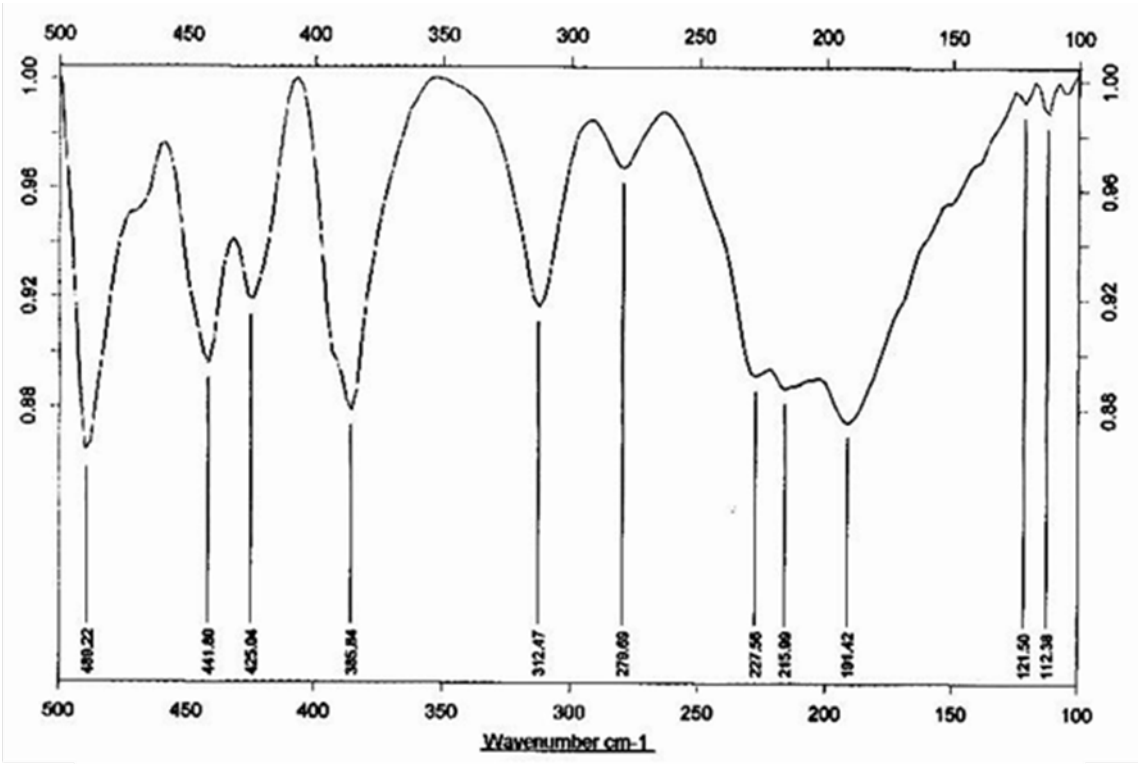
H_2AcbHexim·H_2O



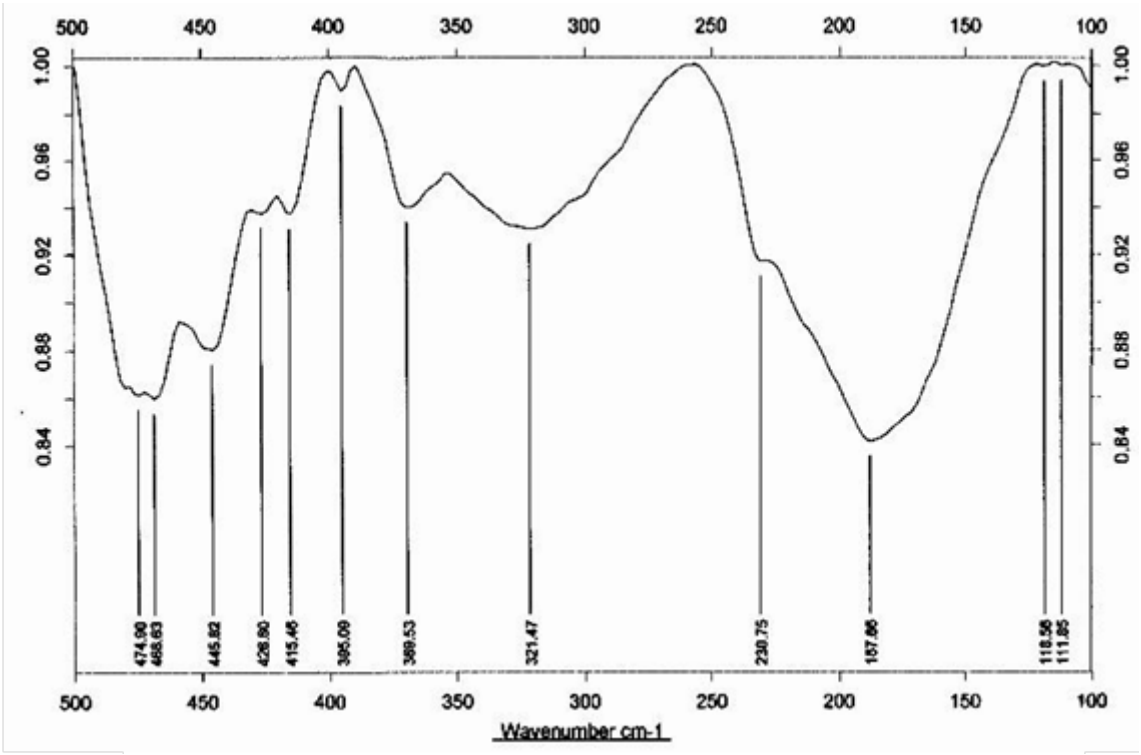
[Cu(HAcbDM)(OAc)]·3H₂O



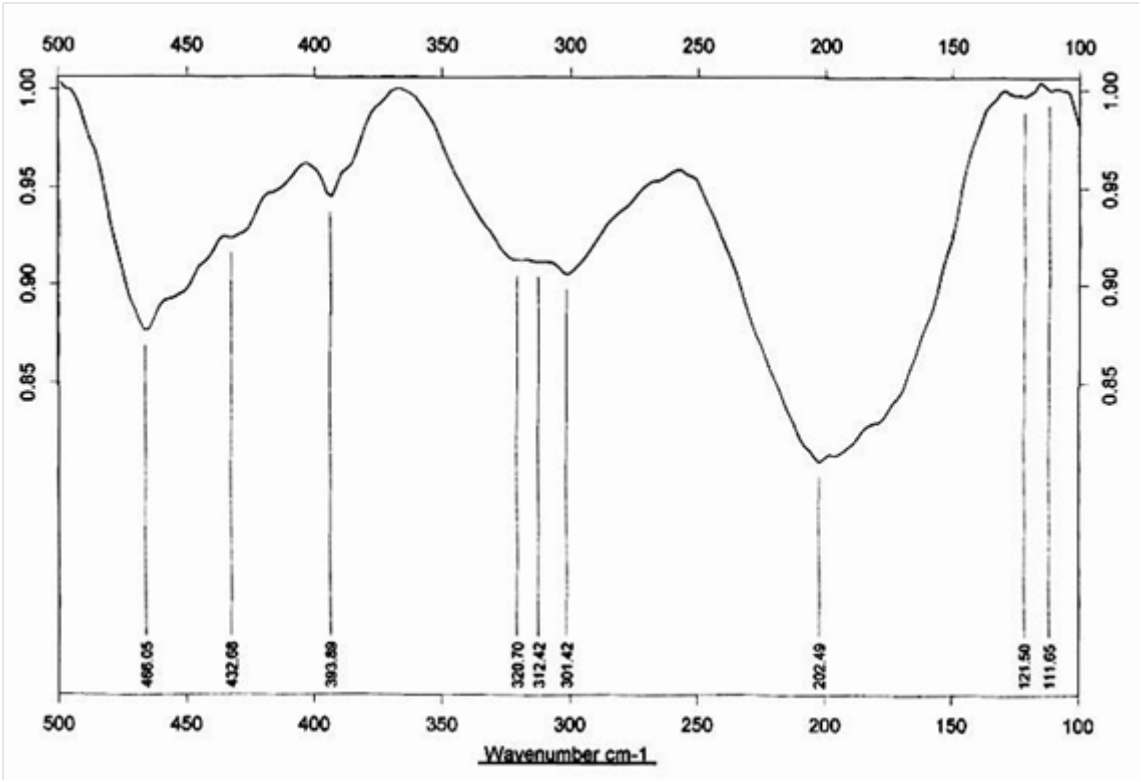
[Cu(HAcbDM)Cl]·1/2EtOH



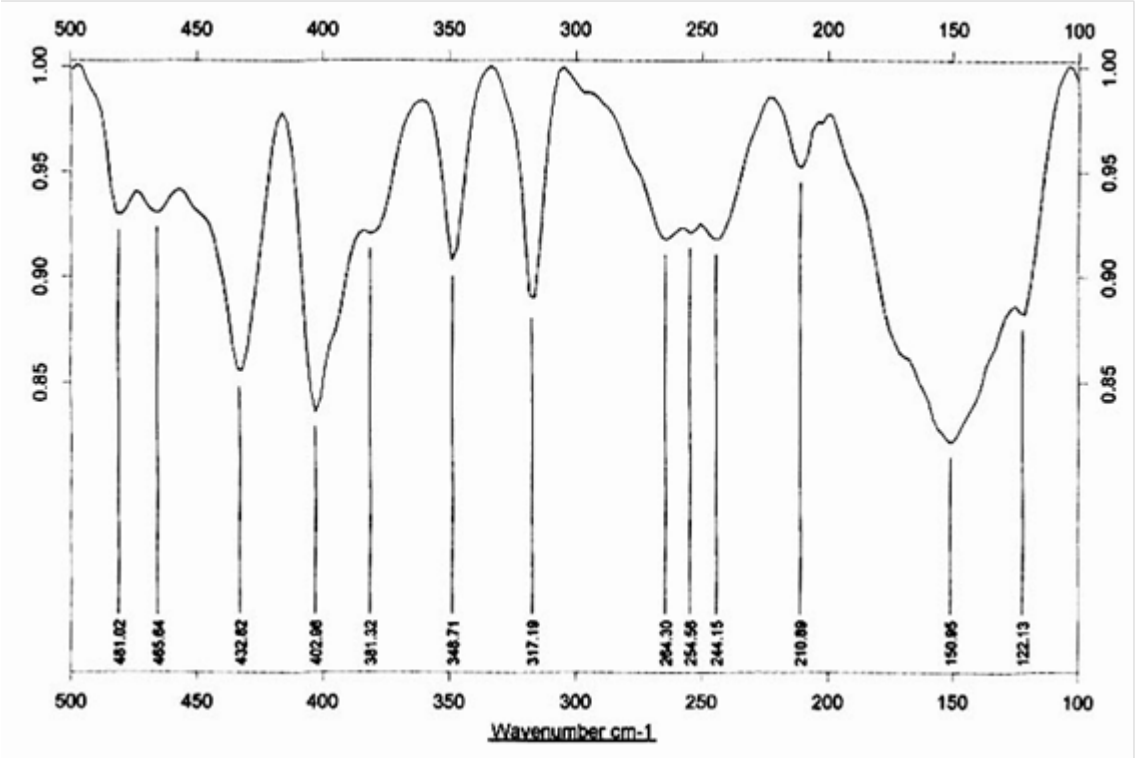
[Cu(HAcbDM)(NO₃)]



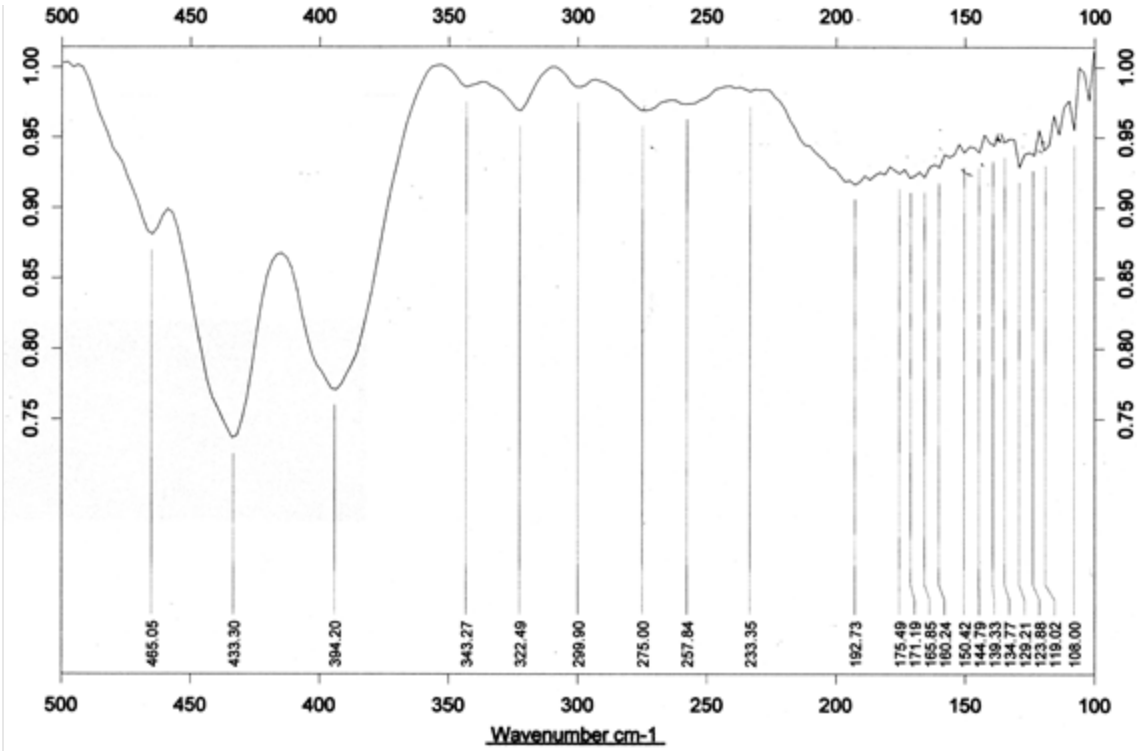
[Cu(HAcbDM)(H₂O)₂]ClO₄



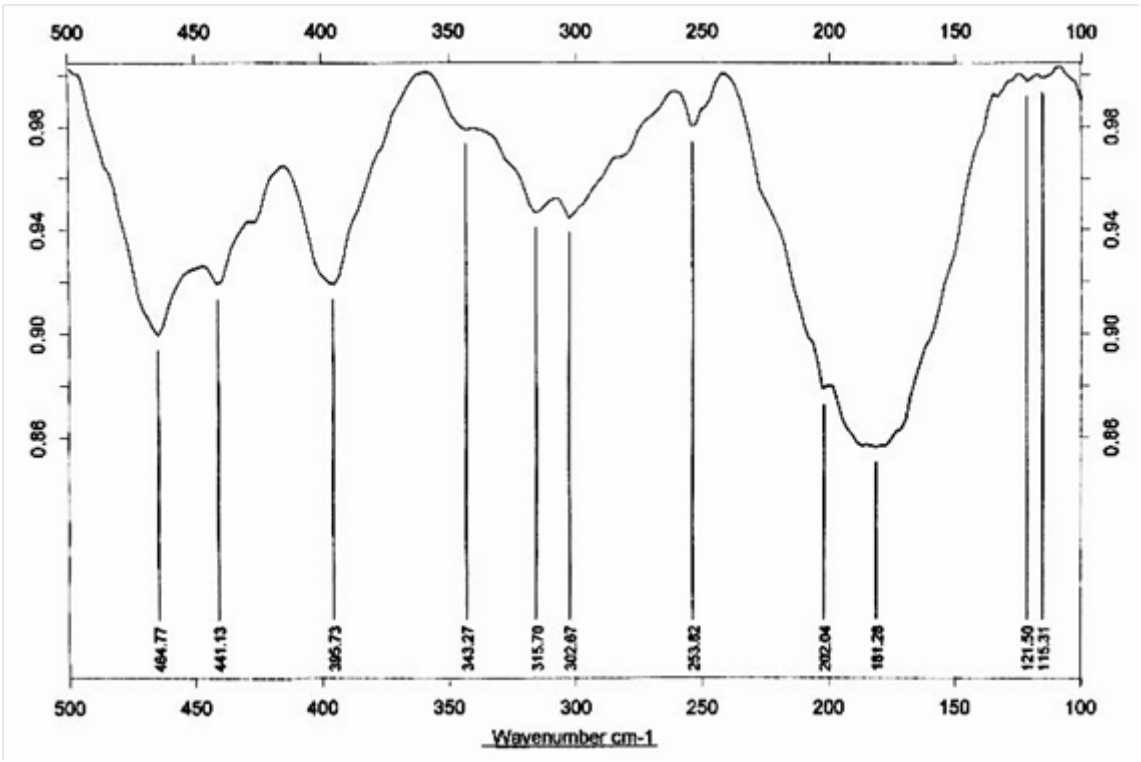
[Cu(HAcbHexim)(OAc)]·5H₂O



[Cu(HAcbHexim)Cl]·1/2EtOH

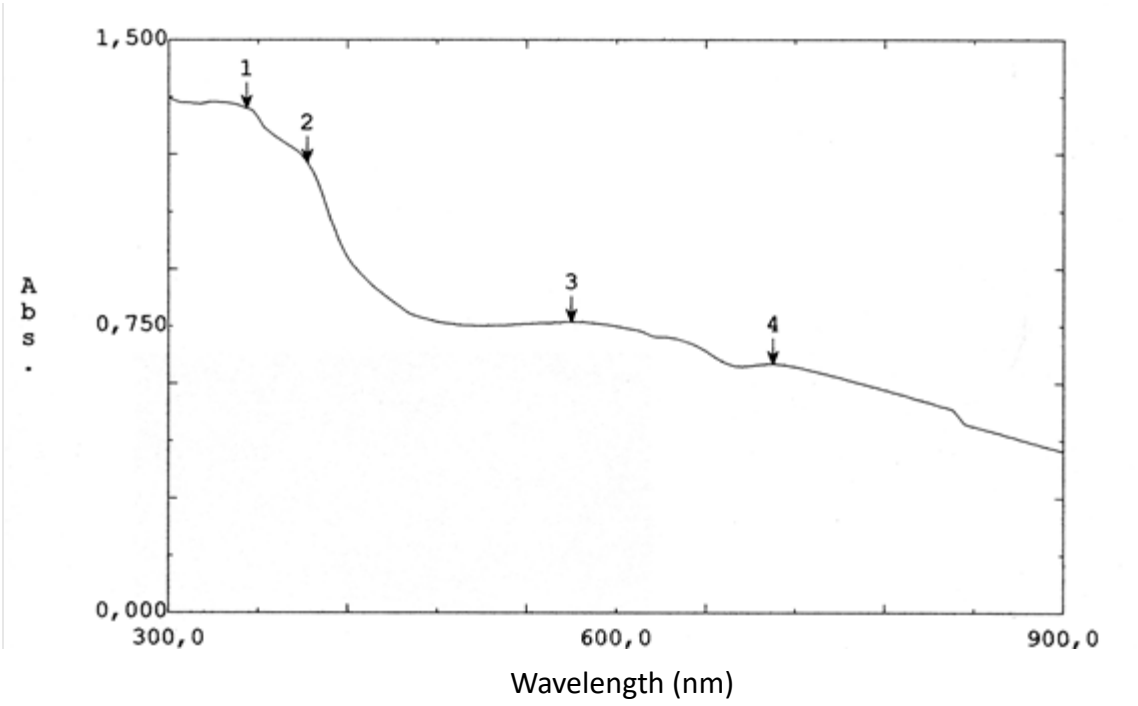


[Cu(HAcbHexim)(NO_3)]·1/2H_2O

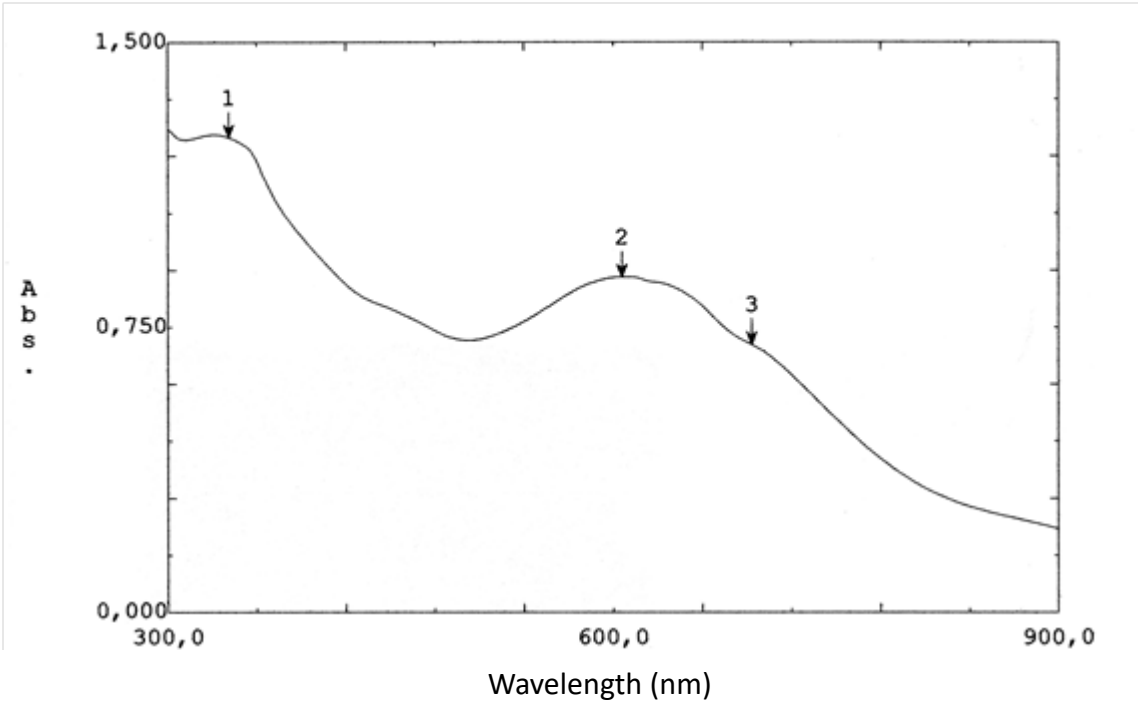


[Cu(HAcbHexim)ClO_4]

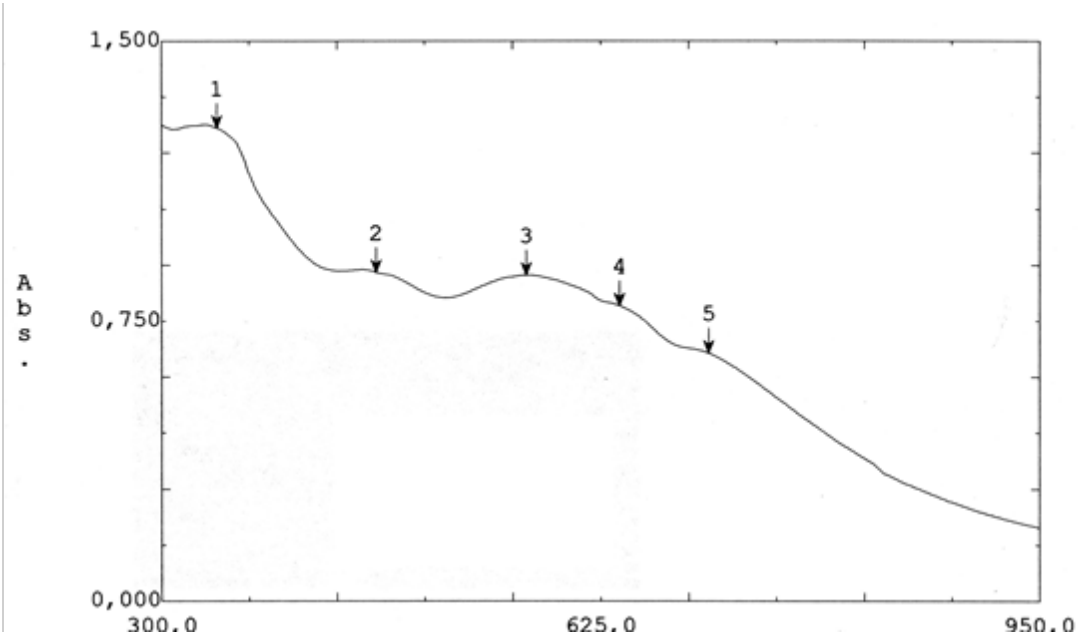
Figure S4. UV-visible Spectra



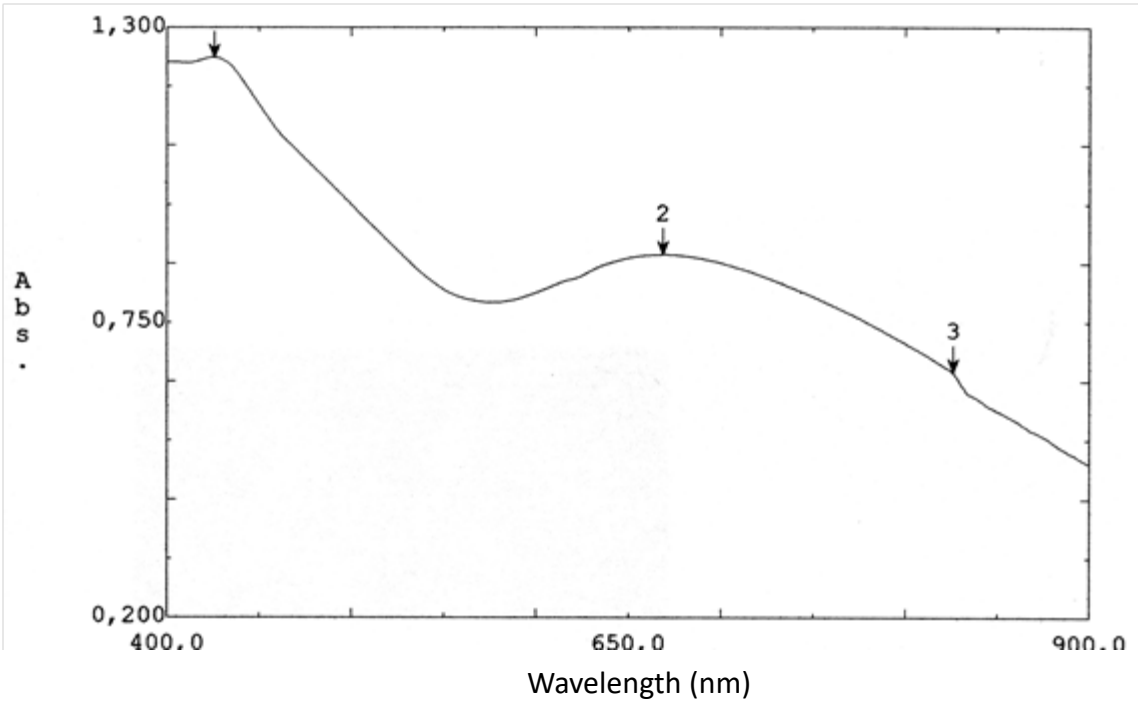
[Cu(HAcbDM)(OAc)]·3H₂O



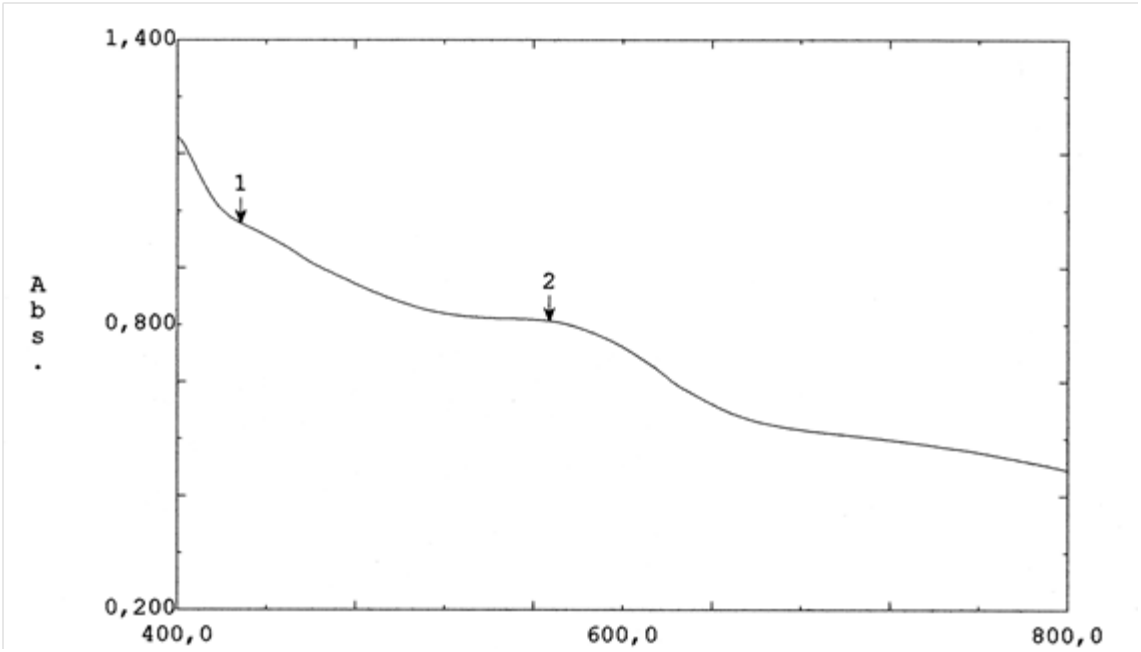
[Cu(HAcbDM)Cl]·1/2EtOH



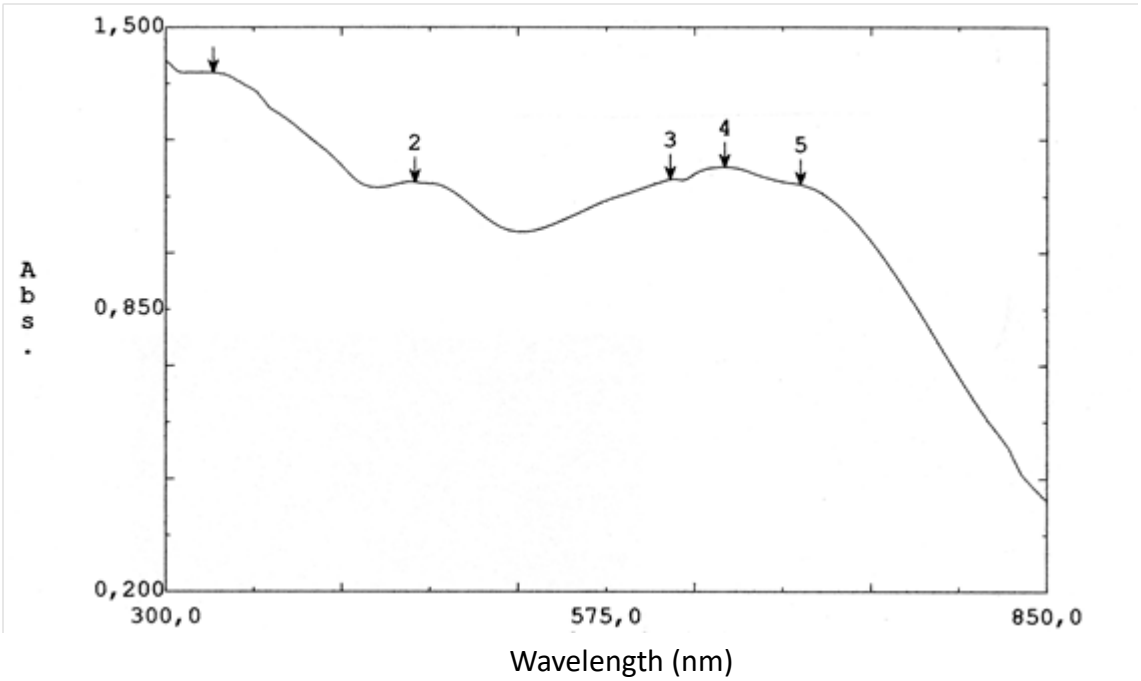
[Cu(HAcbDM)(NO₃)]



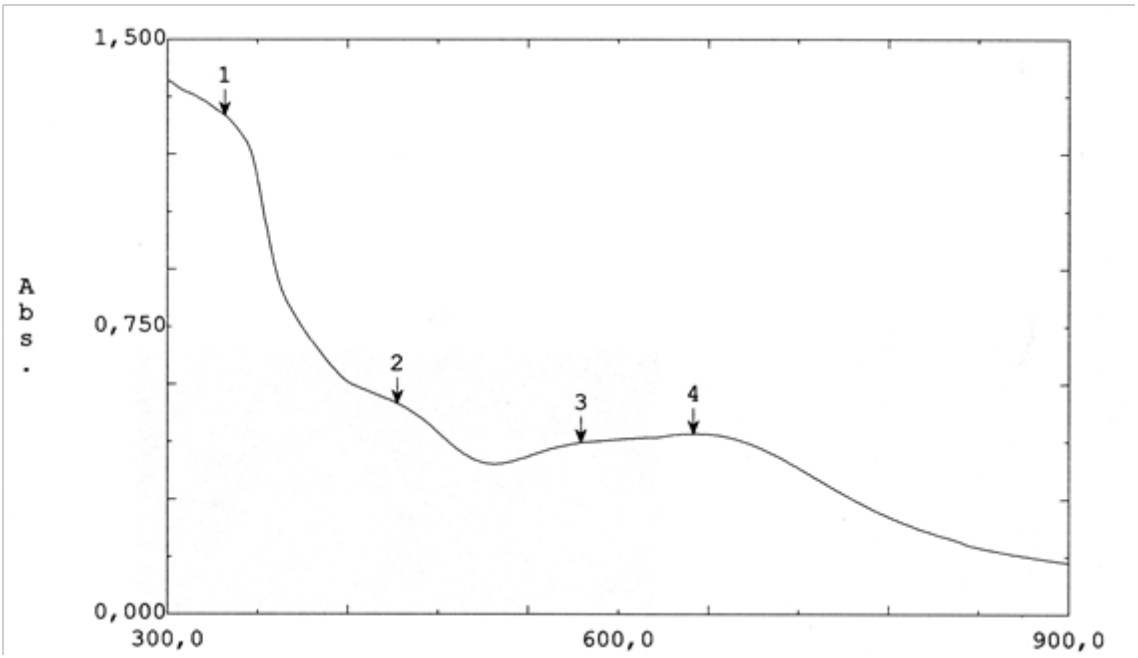
[Cu(HAcbDM)(H₂O)₂]ClO₄



[Cu(HAcbHexim)(OAc)]·5H₂O



[Cu(HAcbHexim)Cl]·1/2EtOH



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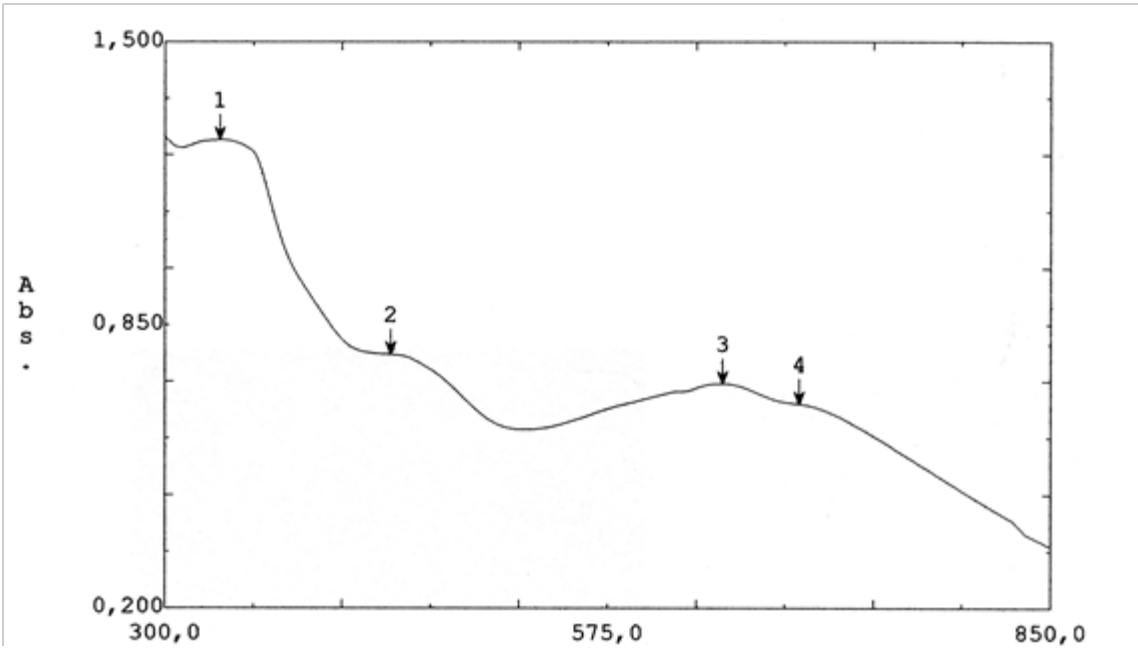
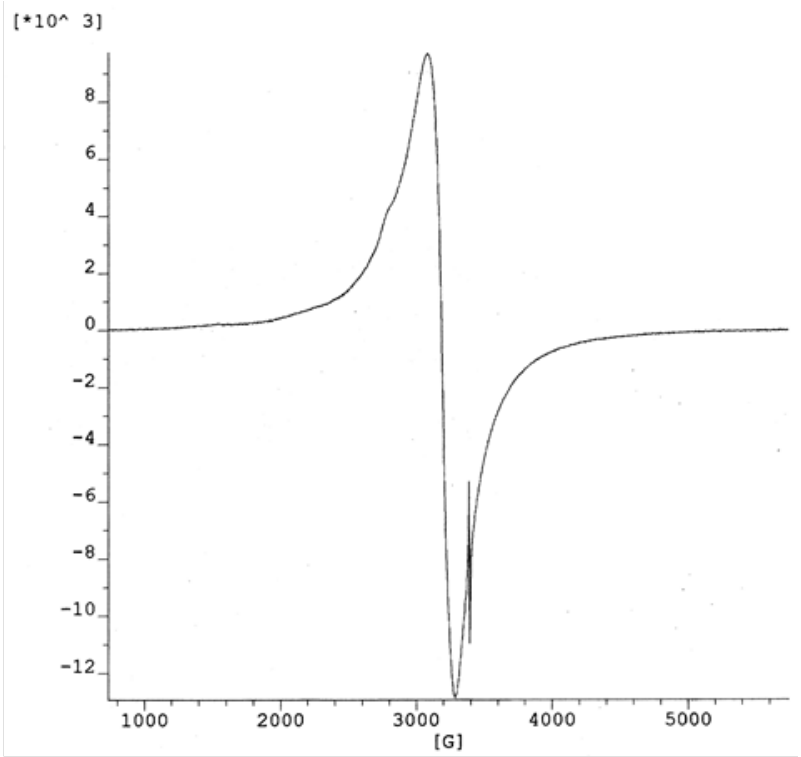
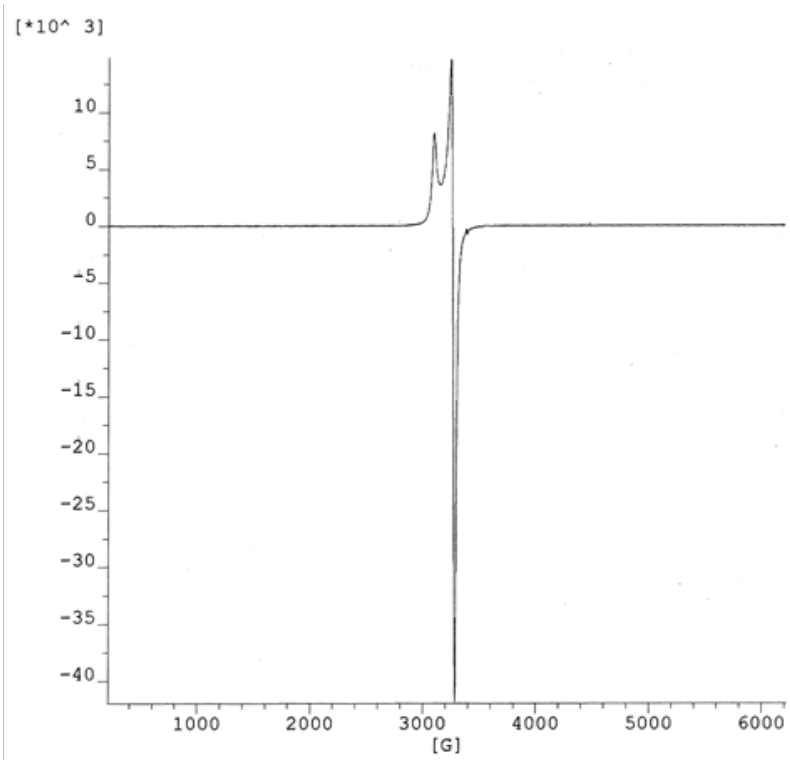


[Cu(HAcbHexim)ClO$_4$]

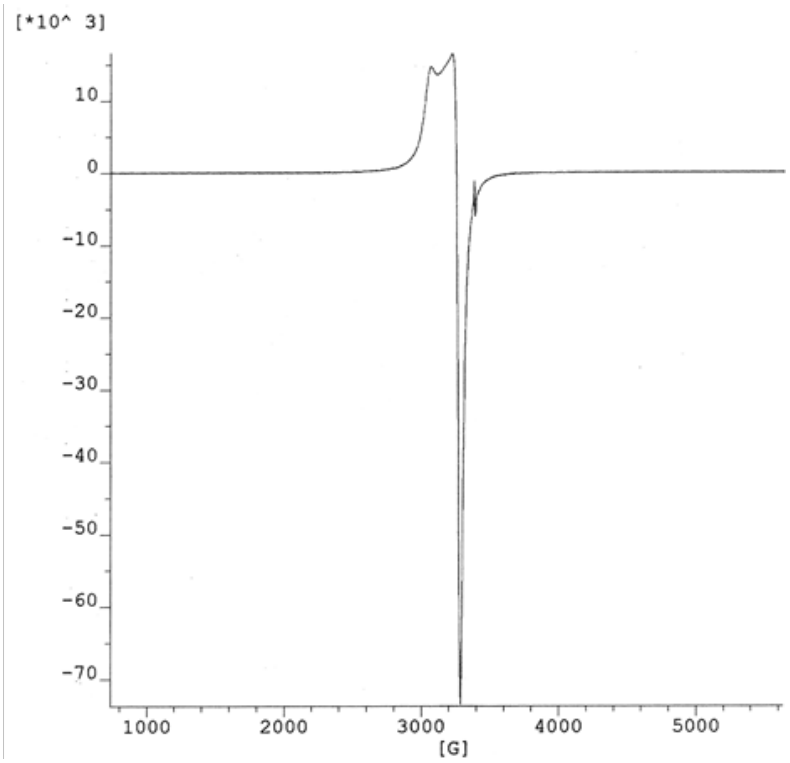
Figure S5. EPR spectra



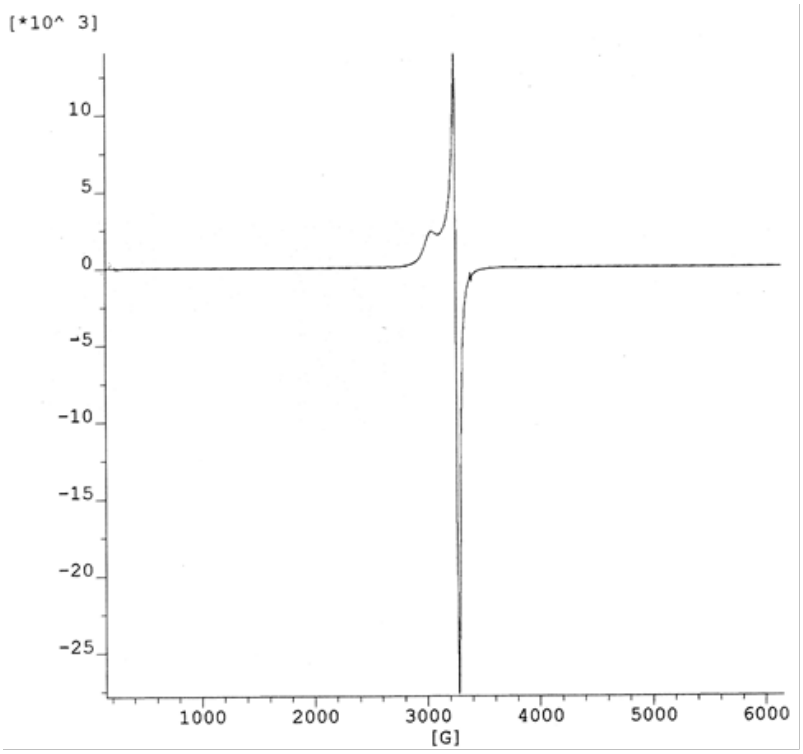
[Cu(HAcbDM)(OAc)]·3H₂O



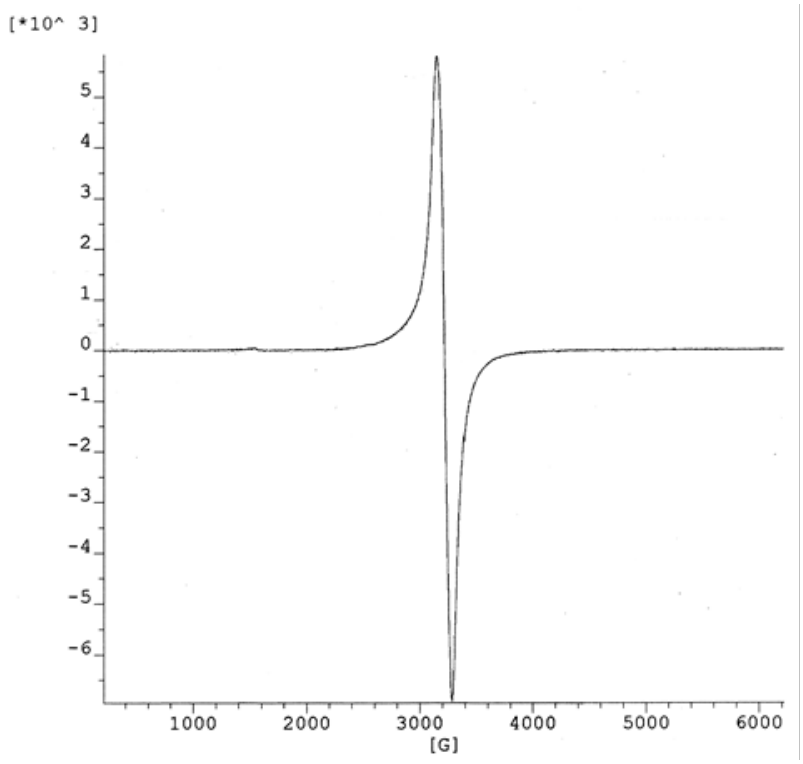
[Cu(HAcbDM)Cl]·1/2EtOH



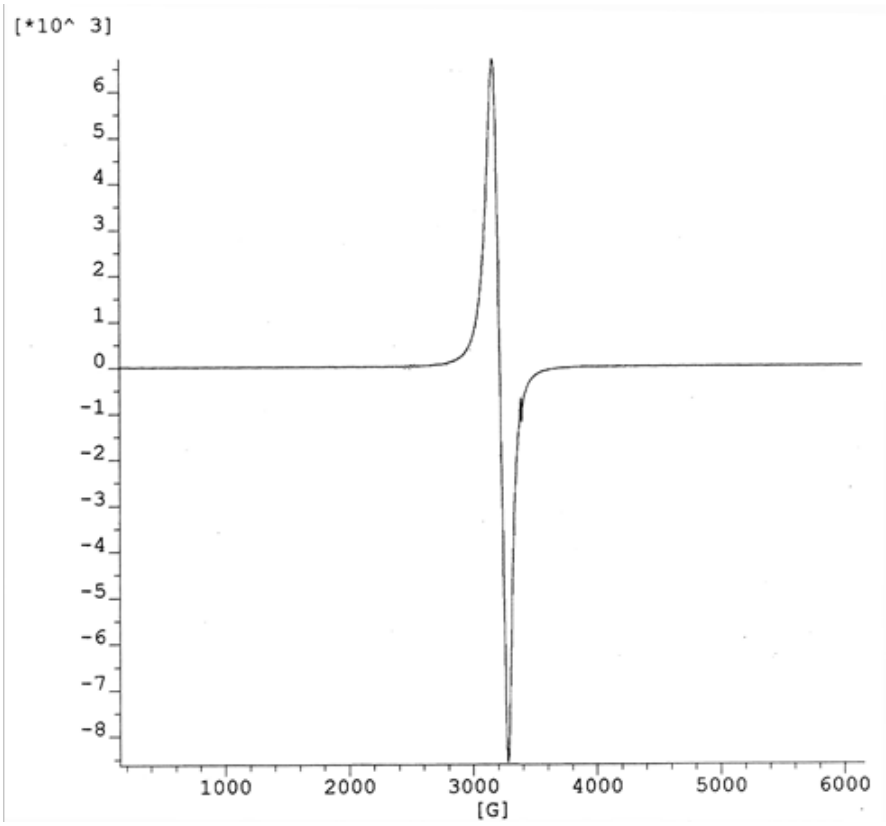
[Cu(HAcbDM)(NO₃)]



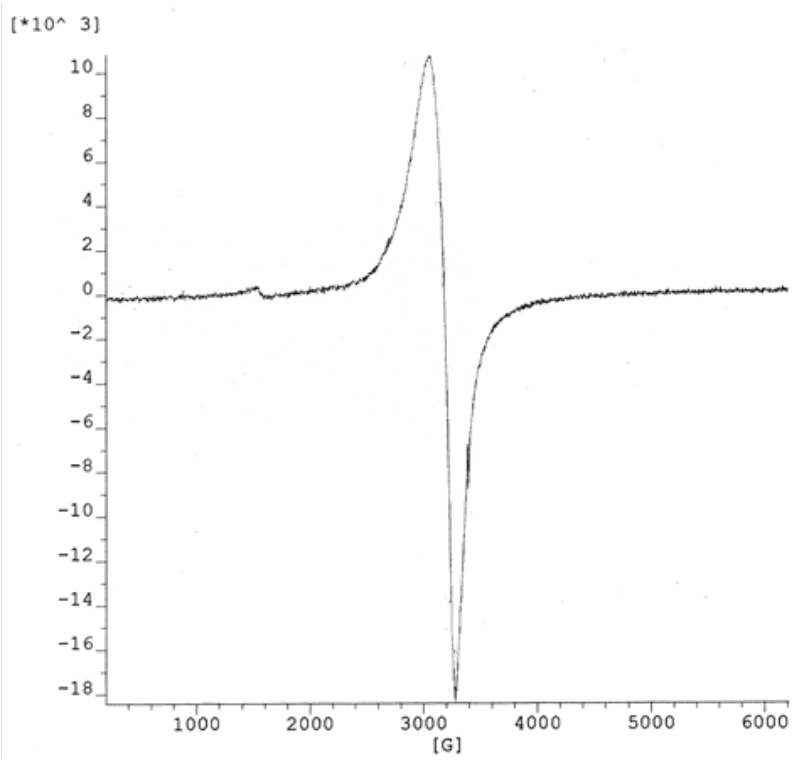
[Cu(HAcbDM)(H₂O)₂]ClO₄



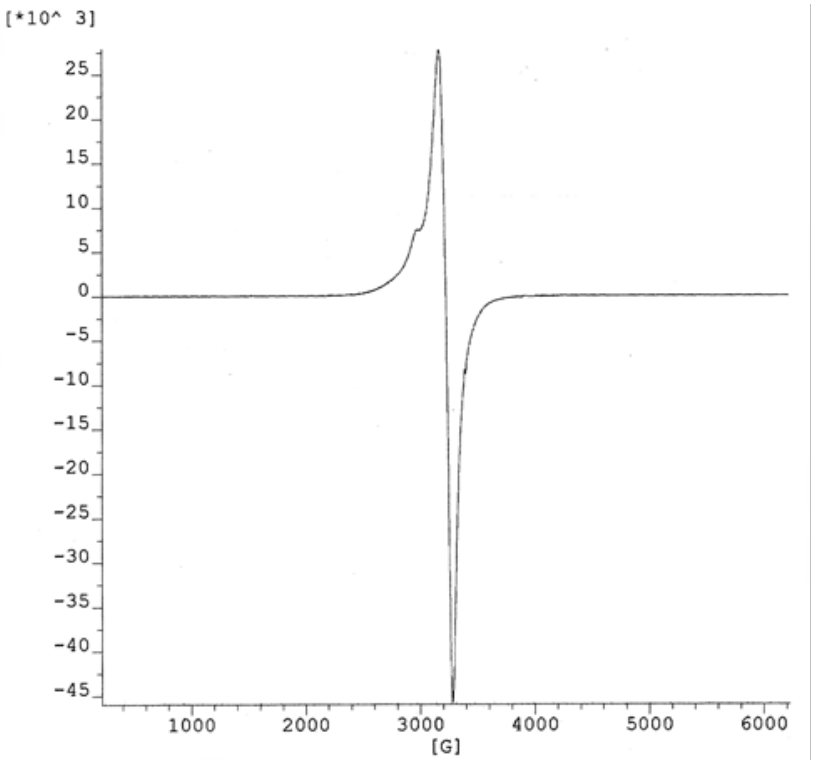
[Cu(HAcbHexim)(OAc)]·5H₂O



[Cu(HAcbHexim)Cl]·1/2EtOH



[Cu(HAcbHexim)(NO₃)]·1/2H₂O



[Cu(HAcbHexim)ClO₄]

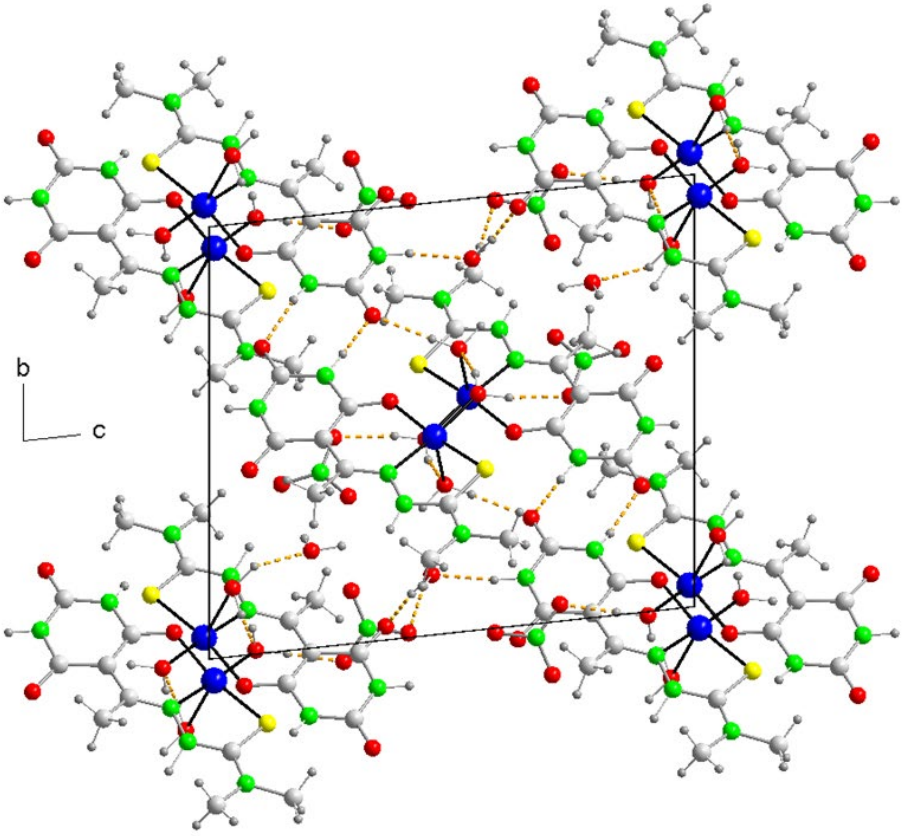


Figure S6. View of the unit cell for **3a** in the "bc" plane, showing the crystal packing. Hydrogen bonds are shows as orange dashed lines.

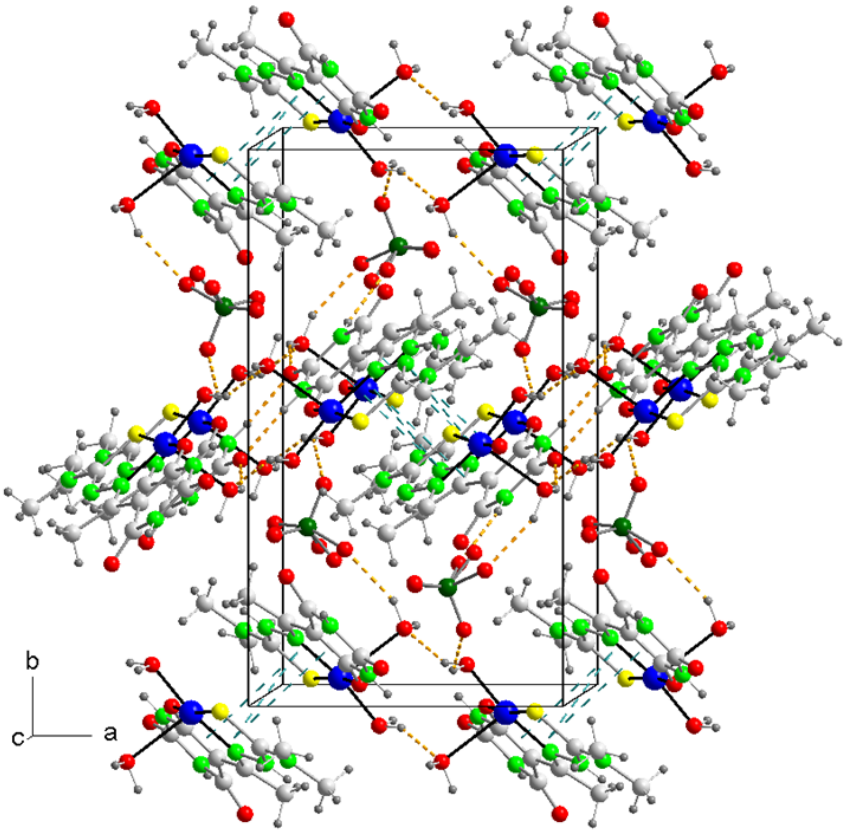


Figure S7. View of the unit cell for **4** in the "bc" plane, showing the crystal packing, the hydrogen bonding (orange dashed lines) and π-π stacking interactions (blue dashed lines).

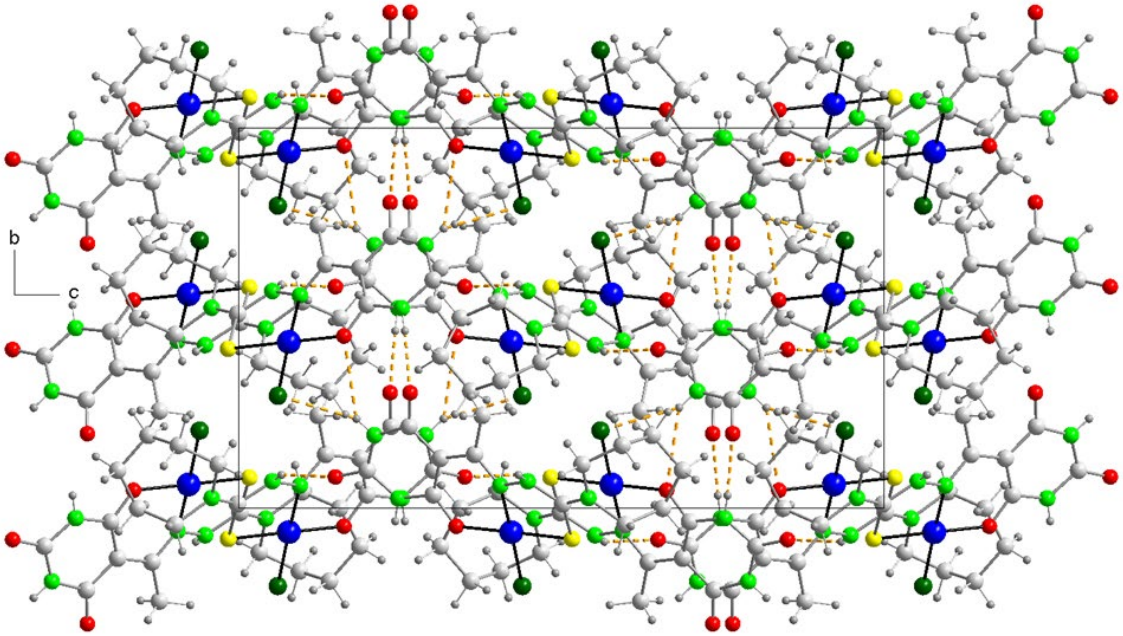
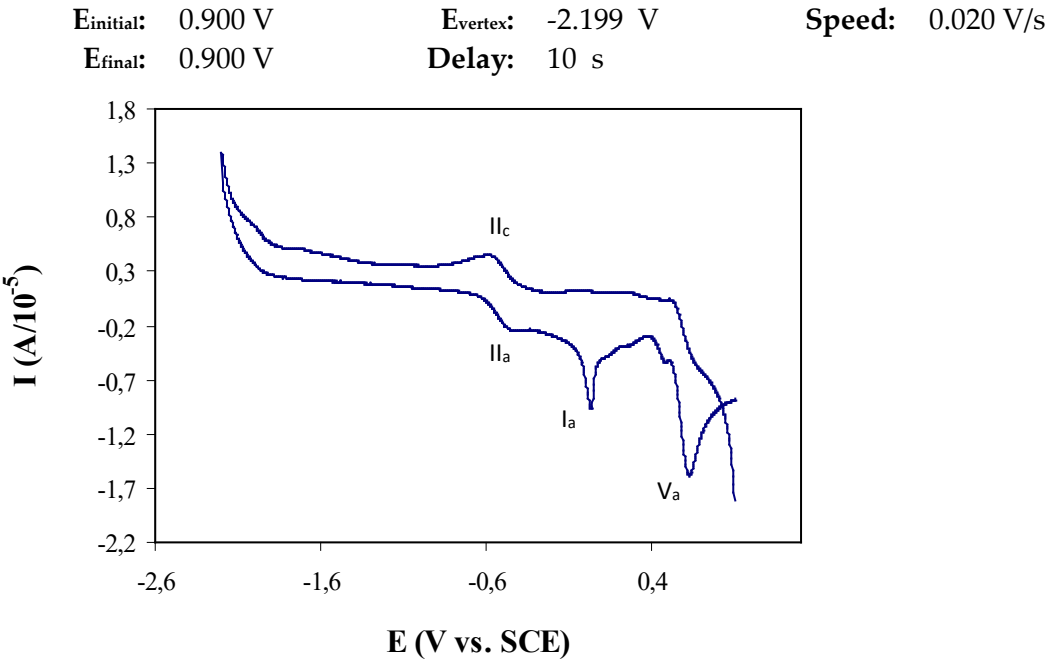


Figure S8. View of the unit cell for **6** in the "bc" plane, showing the crystal packing. Hydrogen bonds are shows as orange dashed lines.

Figure S9. Cyclic voltammograms

[Cu(HAcbDM)(OAc)]·3H₂O (**1**·3H₂O)

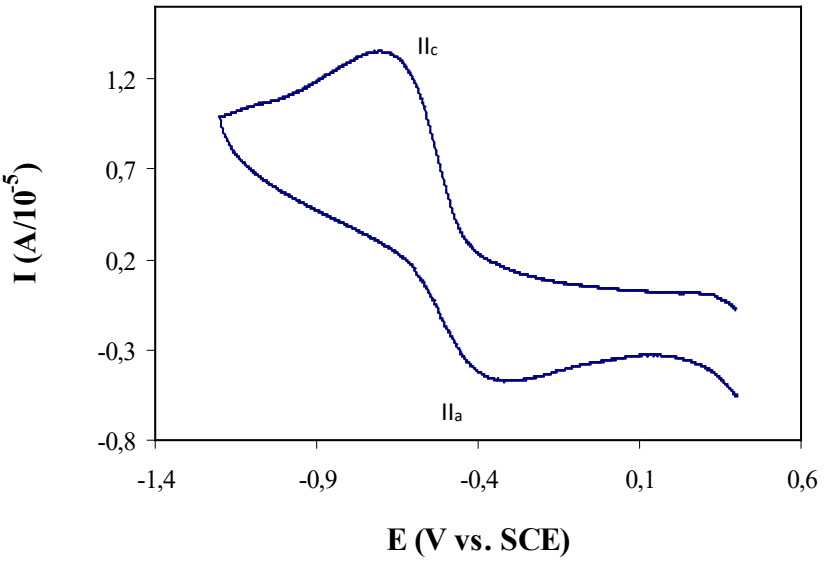


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:		0.033						
II:	-0.582	-0.396	0.186	-0.489	-0.471	0.111	-0.499	-0.553
V:		0.624						

[Cu(HAcbDM)(OAc)]·3H₂O (**1**·3H₂O)

Einitial**:** 0.400 V **E**vertex**:** -1.200 V **Speed:** 0.200 V/s
Efinal**:** 0.400 V **Delay:** 0 s

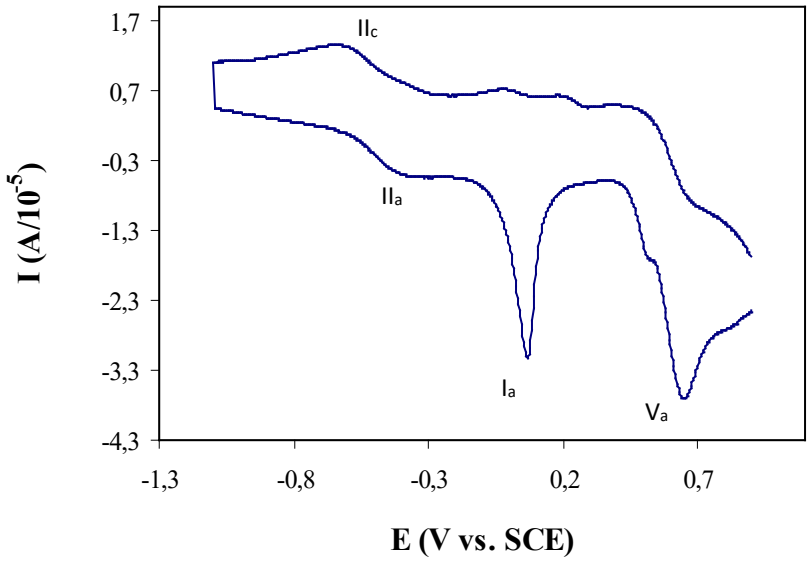


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
II:	-0.708	-0.371	0.337	-0.539	-0.518	0.190	-0.545	-0.679

[Cu(HAcbDM)(OAc)]·3H₂O (**1**·3H₂O)

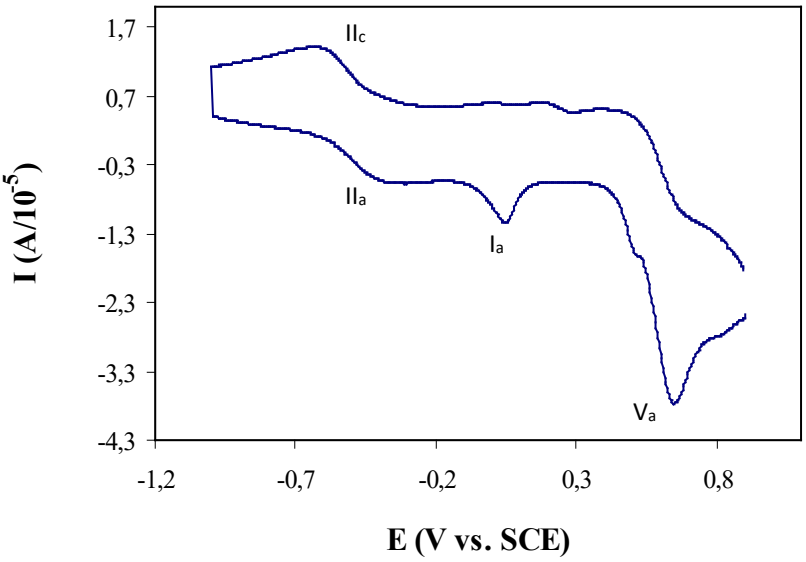
Einitial: 0.900 V **E**vertex: -1.098 V **Speed:** 0.200 V/s
Efinal: 0.900 V **Delay:** 10 s



(No peak potentials have been included)

[Cu(HAcbDM)(OAc)]·3H₂O (**1**·3H₂O)

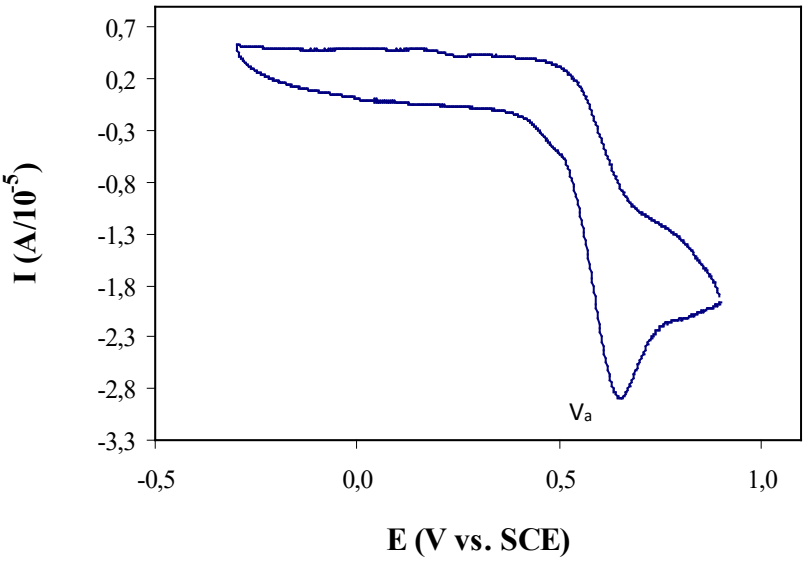
Einitial**:** 0.900 V **E**vertex**:** -0.999 V **Speed:** 0.200 V/s
Efinal**:** 0.900 V **Delay:** 10 s



(No peak potentials have been included)

[Cu(HAcbDM)(OAc)]·3H₂O (**1**·3H₂O)

$E_{initial}$: 0.900 V **E_{vertex}:** -0.300 V **Speed:** 0.200 V/s
E_{final}: 0.900 V **Delay:** 0 s

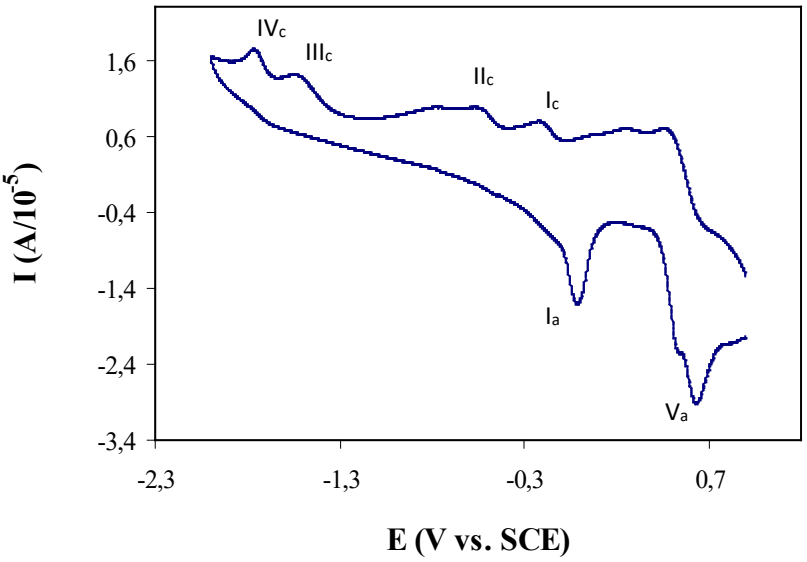


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
V:		0.648						

[Cu(HAcbDM)Cl]·1/2EtOH (**2**·1/2EtOH)

$E_{initial}$: 0.900 V **E_{vertex}:** -2.000 V **Speed:** 0.200 V/s
E_{final}: 0.900 V **Delay:** 0 s

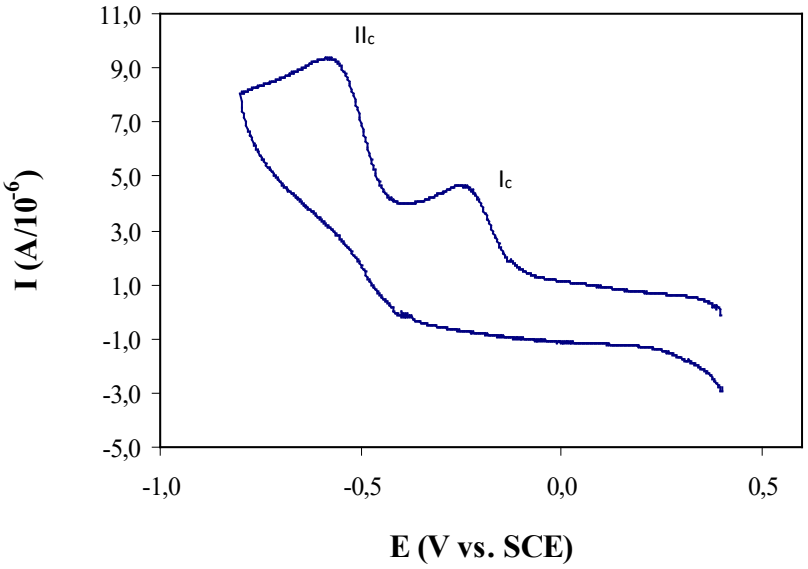


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:	-0.216	-0.015	0.201	-0.115	-0.156	0.060	-0.184	-0.188
II:	-0.558				-0.482	0.076	-0.510	-0.530
III:	-1.534				-1.428	0.106	-1.456	-1.506
IV:	-1.766				-1.714	0.052	-1.741	-1.737
V:		0.631						

[Cu(HAcbDM)Cl]·1/2EtOH (**2**·1/2EtOH)

$E_{initial}$: 0.400 V **E_{vertex}:** -0.800 V **Speed:** 0.200 V/s
E_{final}: 0.400 V **Delay:** 0 s

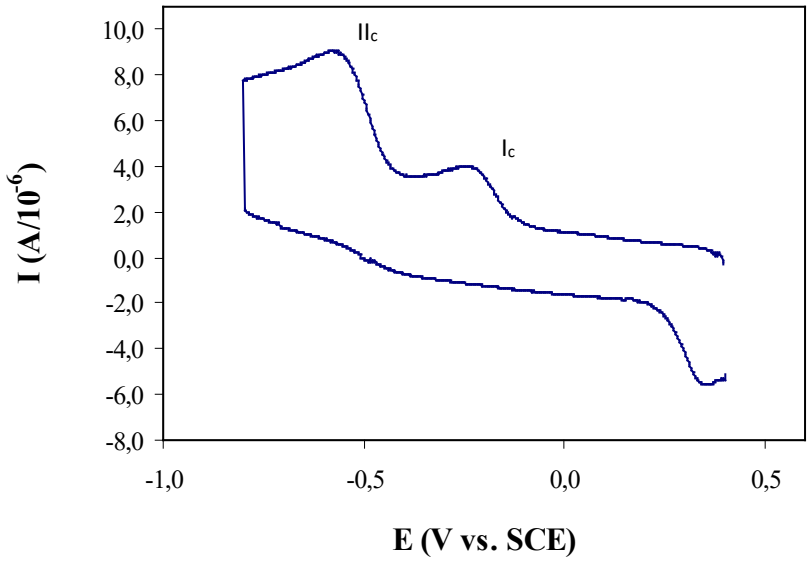


Peak Potentials

System	$(E_P)_c$	$(E_P)_a$	$(E_P)_a - (E_P)_c$	$[(E_P)_a + (E_P)_c]/2$	$(E_{P/2})_c$	$(E_{P/2})_c - (E_P)_c$	$(E_{1/2})_c$	$E^{o'}$
I:	-0.234				-0.170	0.064	-0.197	-0.205
II:	-0.582				-0.494	0.088	-0.521	-0.553

[Cu(HAcbDM)Cl]·1/2EtOH (**2**·1/2EtOH)

$E_{initial}$: 0.400 V **E_{vertex}:** -0.800 V **Speed:** 0.200 V/s
E_{final}: 0.400 V **Delay:** 10 s

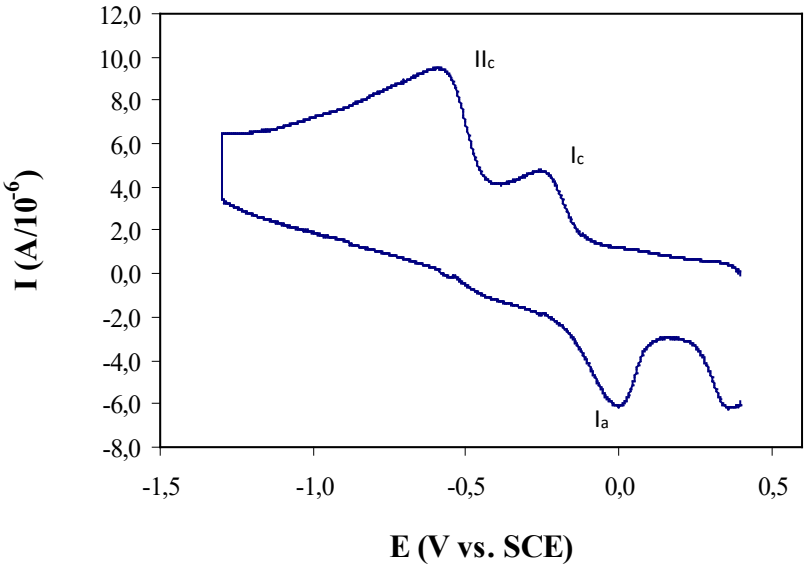


Peak Potentials

System	$(E_P)_c$	$(E_P)_a$	$(E_P)_a - (E_P)_c$	$[(E_P)_a + (E_P)_c]/2$	$(E_{P/2})_c$	$(E_{P/2})_c - (E_P)_c$	$(E_{1/2})_c$	$E^{o'}$
I:	-0.238				-0.168	0.070	-0.195	-0.209
II:	-0.576				-0.490	0.086	-0.517	-0.547

[Cu(HAcbDM)Cl]·1/2EtOH (**2**·1/2EtOH)

$E_{initial}$: 0.400 V **E_{vertex}:** -1.300 V **Speed:** 0.200 V/s
E_{final}: 0.400 V **Delay:** 10 s

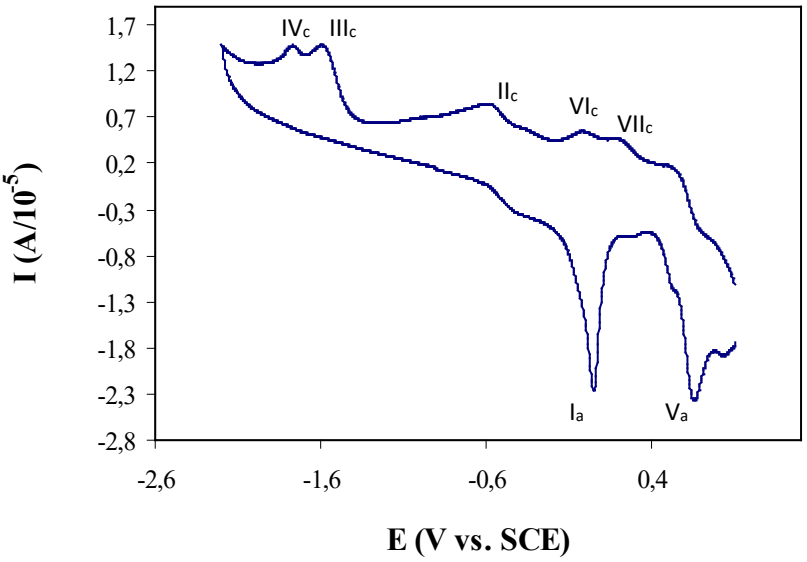


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:	-0.256	-0.007	0.249	-0.131	-0.174	0.082	-0.201	-0.227
II:	-0.588				-0.494	0.094	-0.521	-0.559

[Cu(HAcbDM)(NO$_3$)] (**3**)

E$_{initial}$: 0.900 V **E$_{vertex}$:** -2.199 V **Speed:** 0.200 V/s
E$_{final}$: 0.900 V **Delay:** 0 s

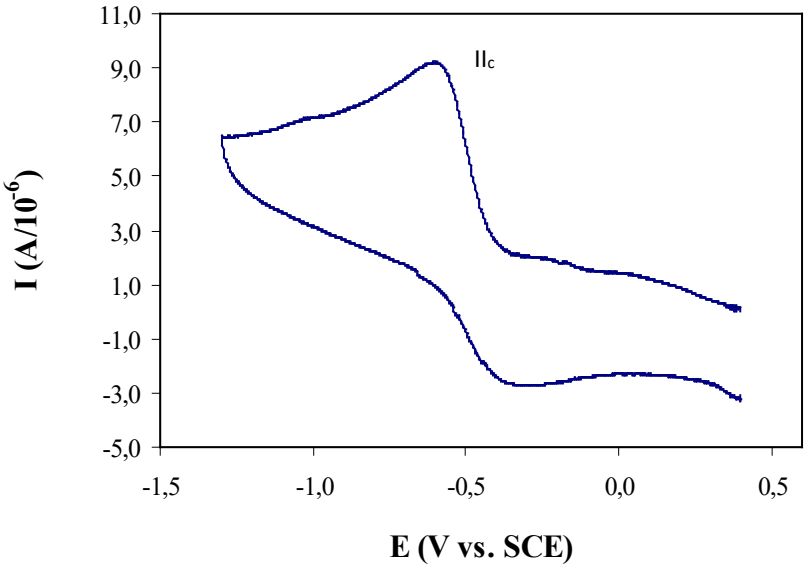


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:		0.048						
II:	-0.597				-0.465	0.132	-0.493	-0.569
III:	-1.593				-1.497	0.096	-1.525	-1.565
IV:	-1.77				-1.71	0.060	-1.738	-1.742
V:		0.651						
VI:	0.20				0.282	0.081	0.254	0.230
VII:	-0.036				0.045	0.081	0.017	-0.007

[Cu(HAcbDM)(NO$_3$)] (**3**)

E$_{initial}$: 0.400 V **E$_{vertex}$:** -1.300 V **Speed:** 0.200 V/s
E$_{final}$: 0.400 V **Delay:** 0 s

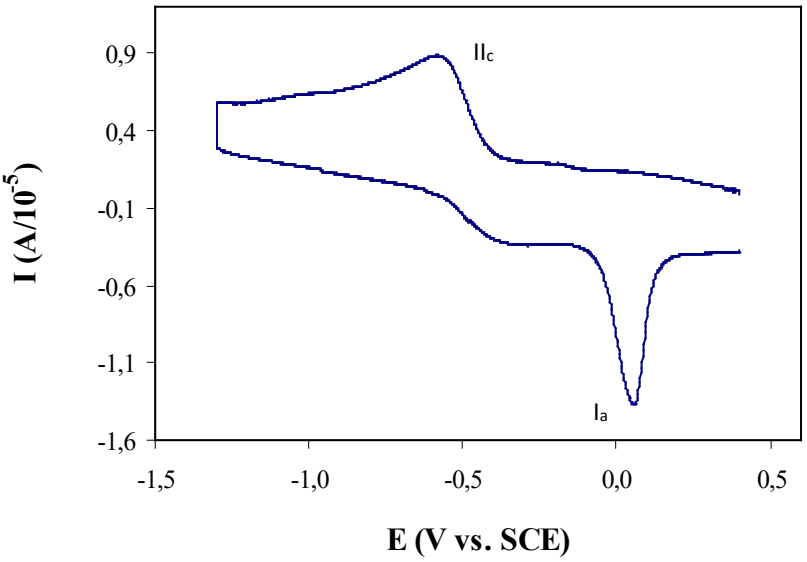


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
II:	-0.596				-0.492	0.104	-0.519	-0.567

[Cu(HAcbDM)(NO3)] (**3**)

Einitial: 0.400 V **Evertex:** -1.300 V **Speed:** 0.200 V/s
Efinal: 0.400 V **Delay:** 10 s

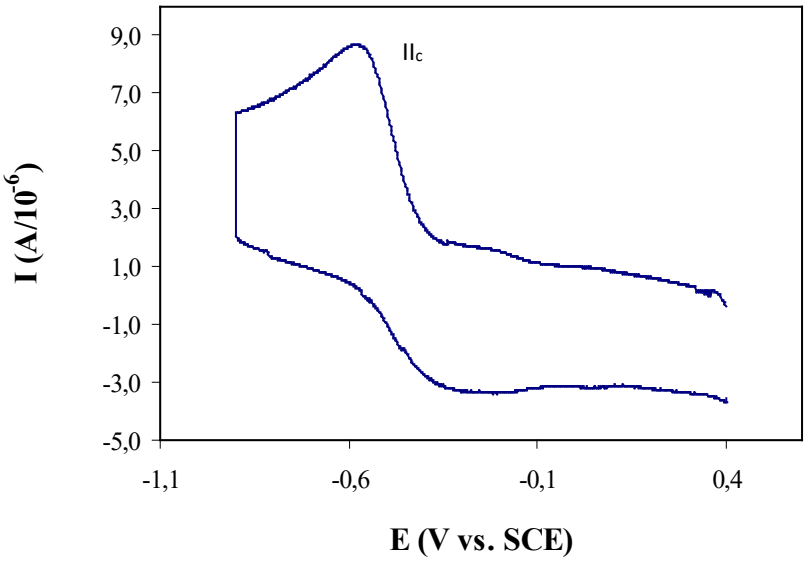


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:		0.057						
II:	-0.580				-0.482	0.098	-0.509	-0.551

[Cu(HAcbDM)(NO3)] (**3**)

Einitial: 0.400 V **Evertex:** -0.900 V **Speed:** 0.200 V/s
Efinal: 0.400 V **Delay:** 10 s

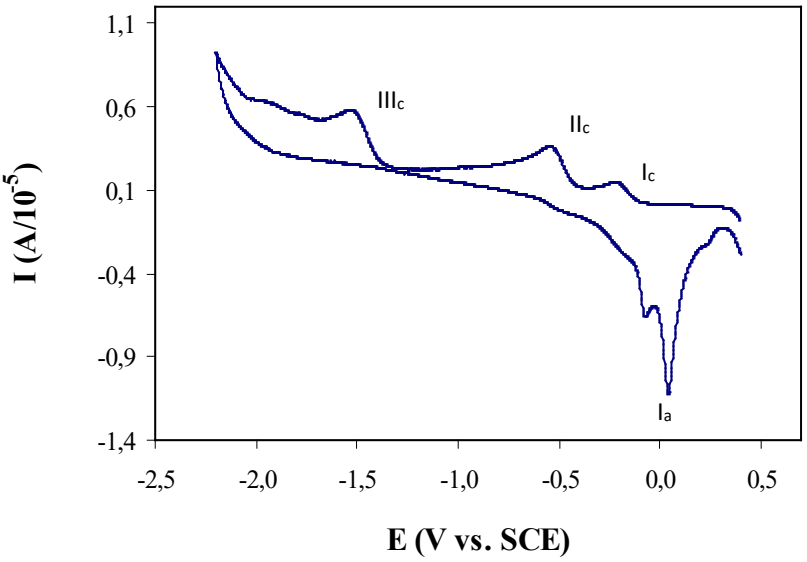


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
II:	-0.580				-0.478	0.102	-0.505	-0.551

[Cu(HAcbHexim)Cl]·1/2EtOH (**6**·1/2EtOH)

$E_{initial}$: 0.400 V **E_{vertex}:** -2.200 V **Speed:** 0.020 V/s
E_{final}: 0.400 V **Delay:** 0 s

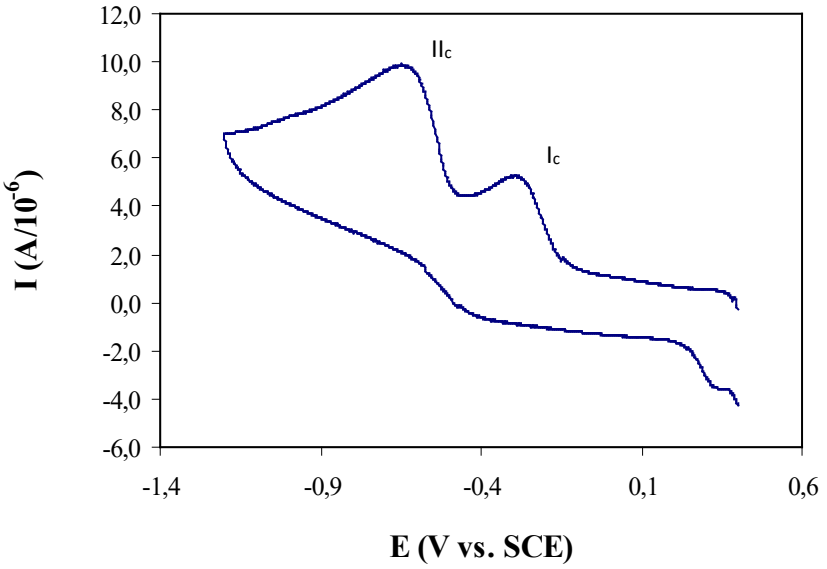


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:	-0.216	0.046	0.262	-0.085	-0.156	0.060	-0.184	-0.188
II:	-0.540				-0.476	0.064	-0.504	-0.511
III:	-1.546				-1.444	0.102	-1.472	-1.518

[Cu(HAcbHexim)Cl]·1/2EtOH (**6**·1/2EtOH)

$E_{initial}$: 0.400 V **E_{vertex}:** -1.200 V **Speed:** 0.200 V/s
E_{final}: 0.400 V **Delay:** 0 s

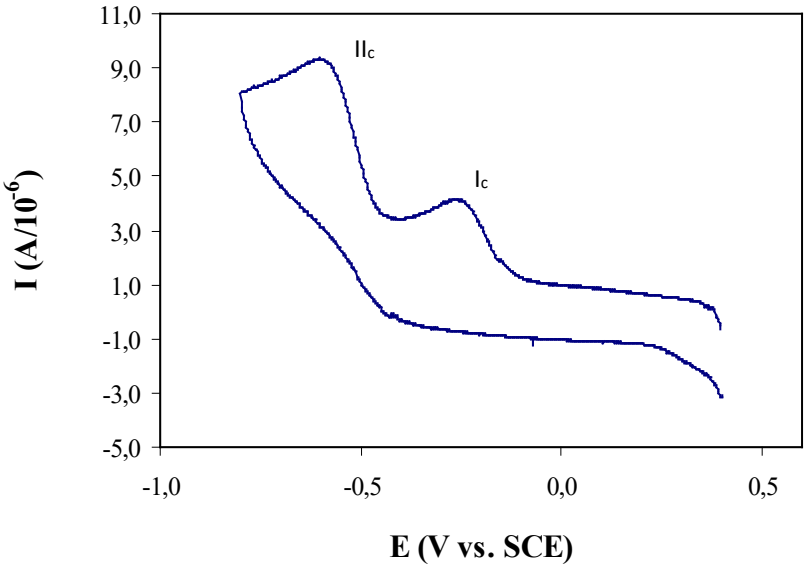


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:	-0.294				-0.206	0.088	-0.233	-0.265
II:	-0.646				-0.544	0.102	-0.571	-0.617

[Cu(HAcbHexim)Cl]·1/2EtOH (**6**·1/2EtOH)

$E_{initial}$: 0.400 V **E_{vertex}:** -0.800 V **Speed:** 0.200 V/s
E_{final}: 0.400 V **Delay:** 0 s

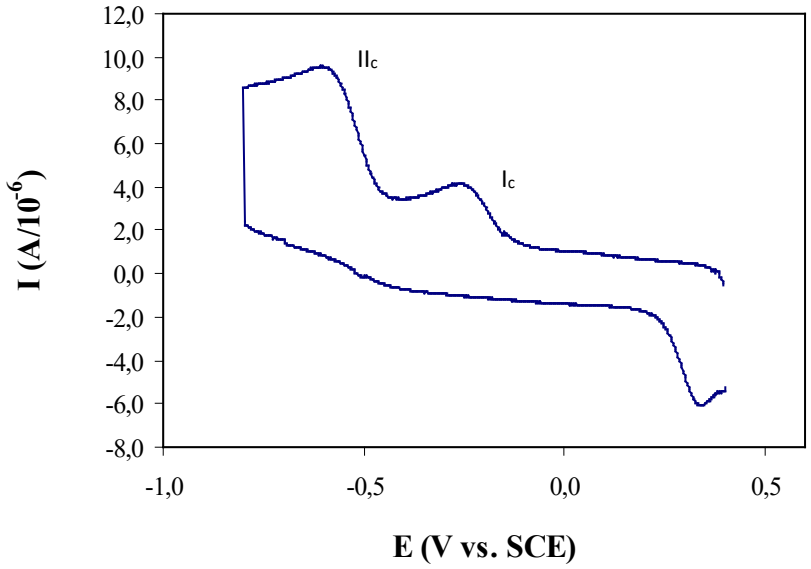


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:	-0.250				-0.184	0.066	-0.211	-0.221
II:	-0.604				-0.516	0.088	-0.543	-0.575

[Cu(HAcbHexim)Cl]·1/2EtOH (**6**·1/2EtOH)

$E_{initial}$: 0.400 V **E_{vertex}:** -0.800 V **Speed:** 0.200 V/s
E_{final}: 0.400 V **Delay:** 10 s

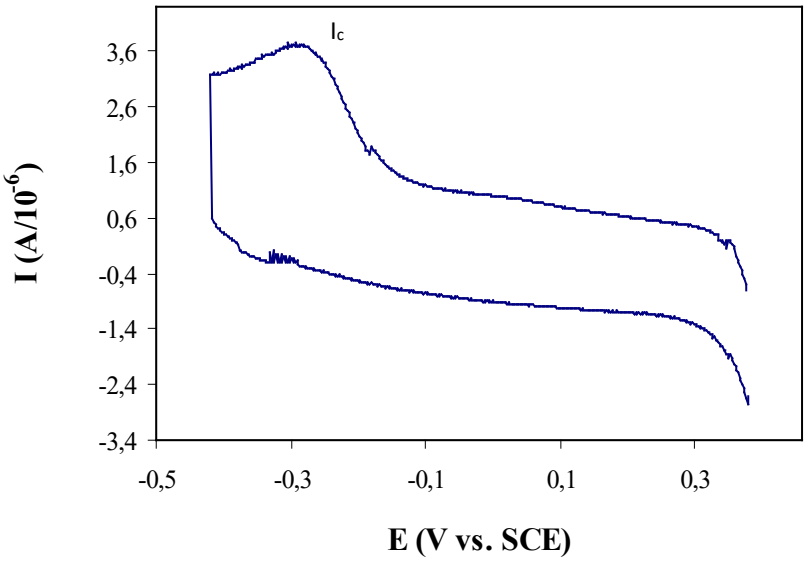


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:	-0.260				-0.186	0.074	-0.213	-0.231
II:	-0.610				-0.516	0.094	-0.543	-0.581

[Cu(HAcbHexim)Cl]·1/2EtOH (**6**·1/2EtOH)

$E_{initial}$: 0.400 V **E_{vertex}:** -0.400 V **Speed:** 0.200 V/s
E_{final}: 0.400 V **Delay:** 10 s

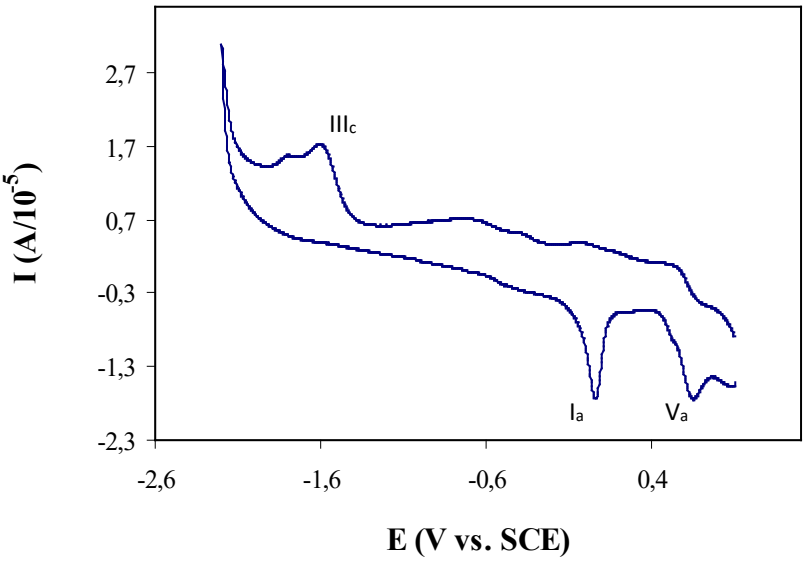


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:	-0.272				-0.192	0.080	-0.219	-0.243

[Cu(HAcbHexim)(NO$_3$)]·1/2H$_2$O (**7**·1/2H$_2$O)

E$_{initial}$: 0.900 V **E$_{vertex}$:** -2.199 V **Speed:** 0.200 V/s
E$_{final}$: 0.900 V **Delay:** 0 s

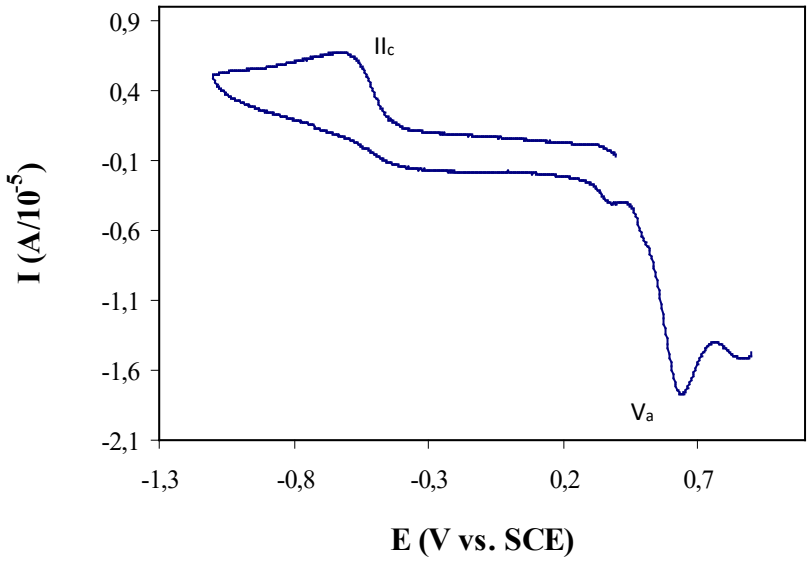


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:		0.060						
III:	-1.602				-1.497	0.105	-1.525	-1.573
V:		0.651						

[Cu(HAcbHexim)(NO3)]·1/2H2O (**7**·1/2H2O)

Einitial: 0.400 V **Evertex:** -1.100 V **Speed:** 0.200 V/s
Efinal: 0.898 V **Delay:** 0 s

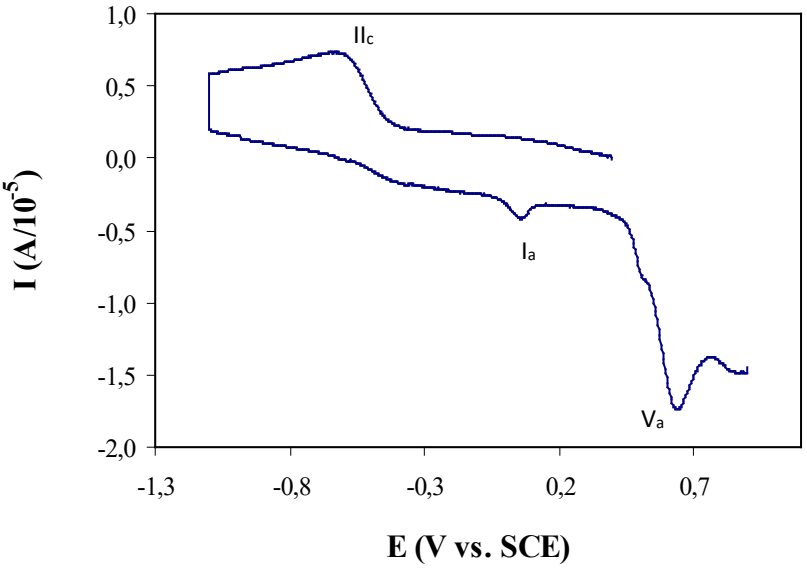


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
II:	-0.620				-0.500	0.120	-0.528	-0.591
V:		0.643						

[Cu(HAcbHexim)(NO$_3$)]·1/2H$_2$O (**7**·1/2H$_2$O)

E$_{initial}$: 0.400 V **E$_{vertex}$:** -1.100 V **Speed:** 0.200 V/s
E$_{final}$: 0.898 V **Delay:** 10 s

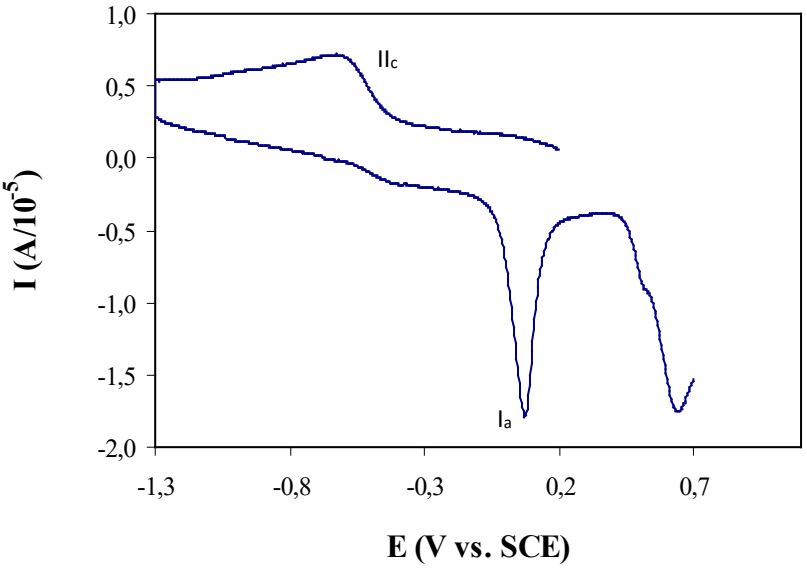


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:		0.058						
II:	-0.632				-0.506	0.126	-0.534	-0.603
V:		0.643						

[Cu(HAcbHexim)(NO$_3$)]·1/2H$_2$O (**7**·1/2H$_2$O)

E$_{initial}$: 0.200 V **E$_{vertex}$:** -1.300 V **Speed:** 0.200 V/s
E$_{final}$: 0.896 V **Delay:** 10 s

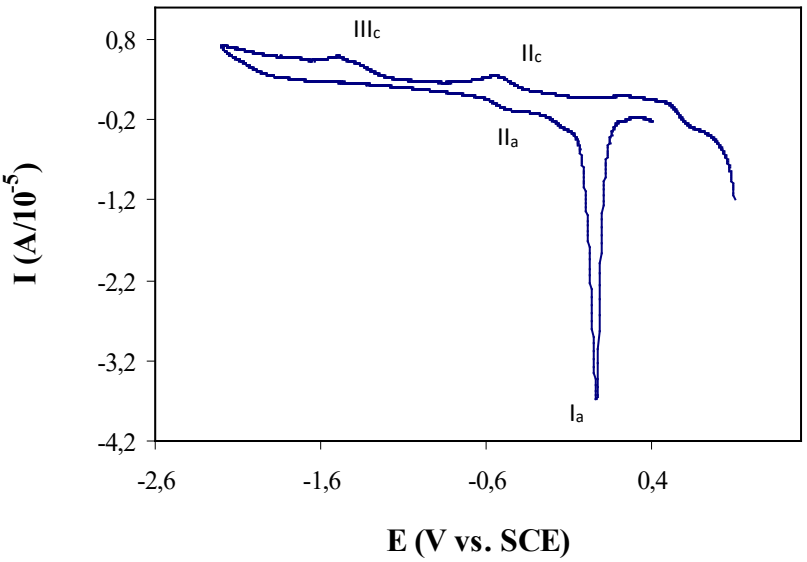


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:		0.074						
II:	-0.628				-0.502	0.126	-0.530	-0.599

[Cu(HAcbHexim)ClO$_4$] (**8**)

E$_{initial}$: 0.900 V **E$_{vertex}$:** -2.200 V **Speed:** 0.020 V/s
E$_{final}$: 0.900 V **Delay:** 0 s

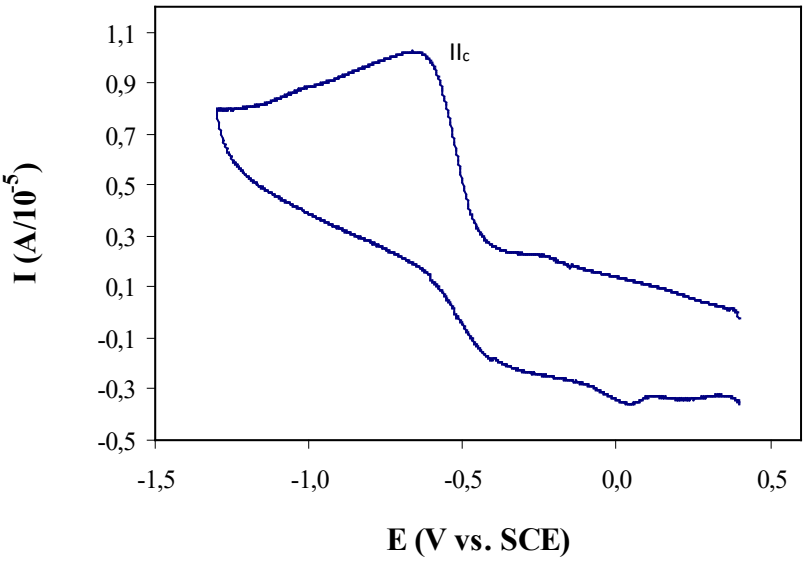


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:		0.066						
II:	-0.55	-0.428	0.122	-0.489	-0.94	-0.390	-0.968	-0.522
III:	-1.492				-1.322	0.170	-1.350	-1.464

[Cu(HAcbHexim)ClO4] (**8**)

Einitial: 0.400 V **Evertex:** -1.300 V **Speed:** 0.200 V/s
Efinal: 0.400 V **Delay:** 0 s

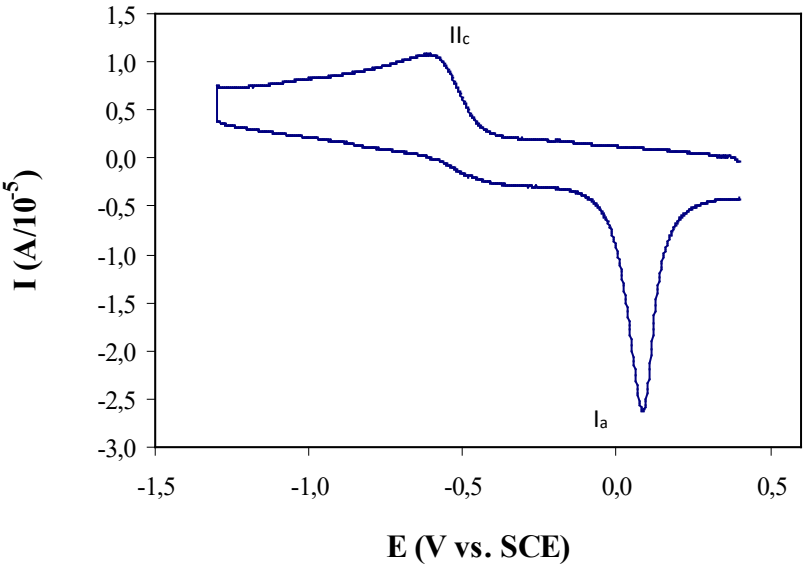


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
II:	-0.662				-0.520	0.142	-0.547	-0.633

[Cu(HAcbHexim)ClO4] (**8**)

Einitial: 0.400 V **Evertex:** -1.300 V **Speed:** 0.200 V/s
Efinal: 0.400 V **Delay:** 10 s

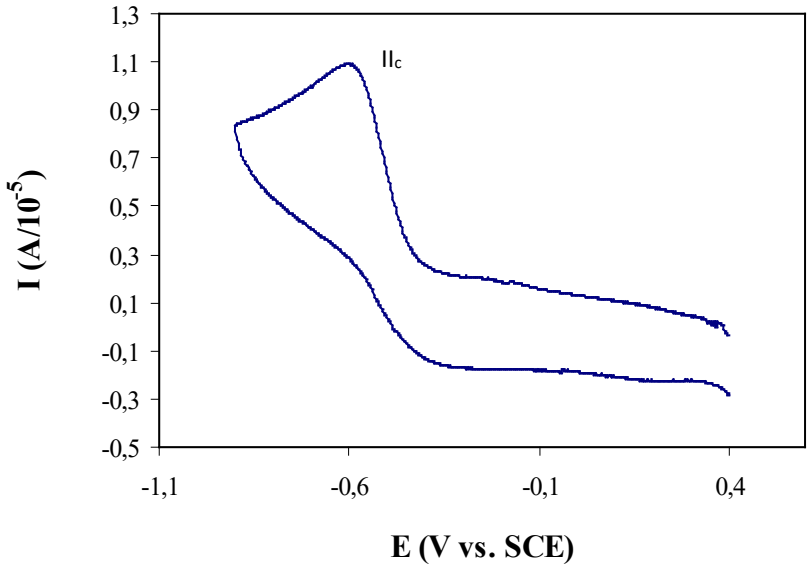


Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
I:		**0.085**						
II:	**-0.604**				**-0.506**	0.098	-0.534	-0.576

[Cu(HAcbHexim)ClO4] (**8**)

Einitial: 0.400 V **Evertex:** -0.900 V **Speed:** 0.200 V/s
Efinal: 0.400 V **Delay:** 0 s



Peak Potentials

System	$(E_p)_c$	$(E_p)_a$	$(E_p)_a - (E_p)_c$	$[(E_p)_a + (E_p)_c]/2$	$(E_{p/2})_c$	$(E_{p/2})_c - (E_p)_c$	$(E_{1/2})_c$	$E^{o'}$
II:	-0.604				-0.502	0.102	-0.529	-0.575