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Table S1. Characteristic IR bands (cm^{-1}) of phthalocyaninato copper complexes **1–6** with 2 cm^{-1} resolution.

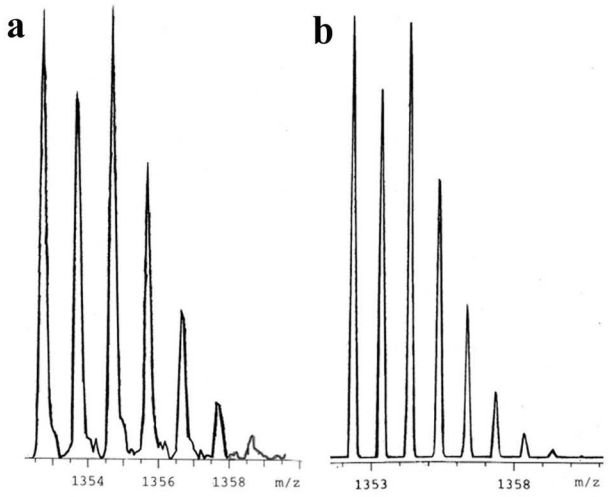
Compound 1 (CuA_4)	Compound 2 (CuA_3B)	Compound 3 (CuAABB)	Compound 5 ($CuAB_3$)	Assignment
2916s	2918s	2918s	2918m	C-H stretching (-CH_2/-CH_3-, asym)
2856m	2857m	2857m	2873m	C-H stretching (-CH_3, sym)
1771w				
1700m				
	1636m	1631s	1630sh	benzene stretching
	1607w	1610sh	1607m	benzene stretching
1567w				
	1509w	1508w	1511w	coupling of pyrrole and aza stretching
			1493s	
1489m	1485m	1484m	1475s	pyrrole and aza stretching
1440s	1449m	1449m	1450s	C=C stretching (thiophene)
1397w	1400w	1400w	1402w	isoindole stretching
1384m	1384w	1384w	1381w	C-H bending (-CH_3, sym)
1349w	1352w	1354w	1357m	C-H bending (-CH_3, sym)
1325w	1333w	1333w		pyrrole stretching
1300w	1303w	1303w	1300sh	Aza stretching
	1280w	1280w	1281s	ArC-O-C stretching(asym)
		1250w	1252w	
1231w	1232w	1233w	1235sh	
1205w	1213w	1213w	1207w	C-H bend
1155m	1154m	1154w		
1110s	1117s	1117s	1119s	ispindole breathing
	1092sh	1090sh	1090sh	C-C stretching
	1054m	1054w	1054m	C-H bending
975s	973s	973m	978m	C-C and C-H bending(-CH_3)
	938w	940w	940m	
908w	905w	907w		Cu-N stretching
867w	867w	870	866w	Coupling of aza stretching
829s			820w	

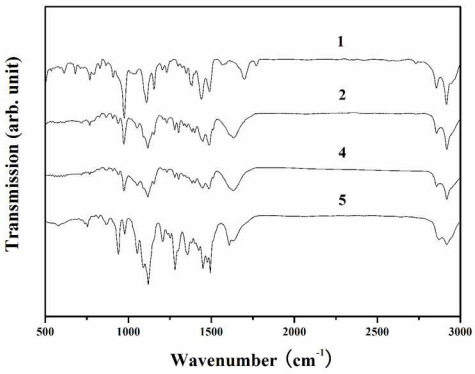
769w	767w	767w	754w	Pc stretching
729w	737w	734w	738sh	
714w	717w	717w	715w	C-H wag
681w				
613w	617w	619w	619w	Pc breathing
	570w		580w	
502m	508w			
467w	474w	467w	476w	C=C-S stretching

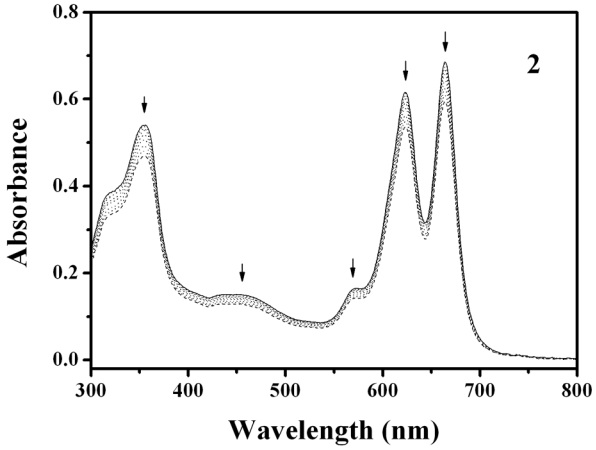
Figure S1. (a) Experimental and (b) simulated isotopic pattern for the molecular ion of compound **4** shown in the MALDI-TOF mass spectrum.

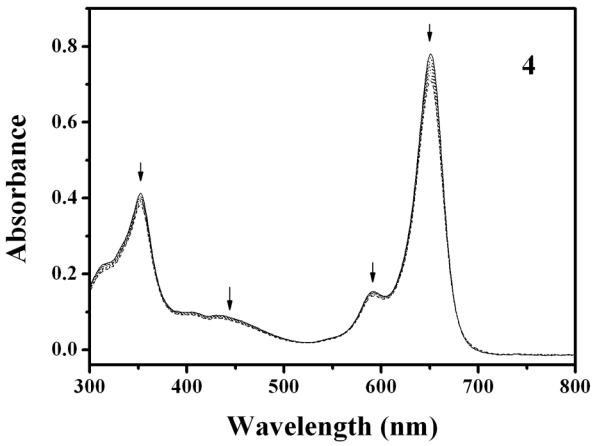
Figure S2. IR spectrum of compound **1**, **2**, **4** and **5** in the region of 500-3000 cm^{-1} with 2 cm^{-1} resolution.

Figure S3. Changes in absorption spectra of CuA_3B (**2**) and CuAABB (**4**) in $CHCl_3$ upon titration with CH_3COOK in $CHCl_3$/MeOH (4:1, v/v). Arrows indicate the direction of the spectral changes. The final spectra were obtained when [CH_3COOK]/[compound] = 3.0.


a
b
1354
1356
1358
m/z
1353
1358
m/z


Transmission (arb. unit)
1
2
4
5
500
1000
1500
2000
2500
3000
Wavenumber (cm-1)


2
Absorbance
Wavelength (nm)
0.0
0.2
0.4
0.6
0.8
300
400
500
600
700
800


4
Absorbance
Wavelength (nm)
0.0
0.2
0.4
0.6
0.8
300
400
500
600
700
800