

Supplementary information

Enhancement of Electroluminescence in Zirconium Poly Carboxylic Acid-Based Light Emitting Diodes by Bathophenanthroline Ligand

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S1:

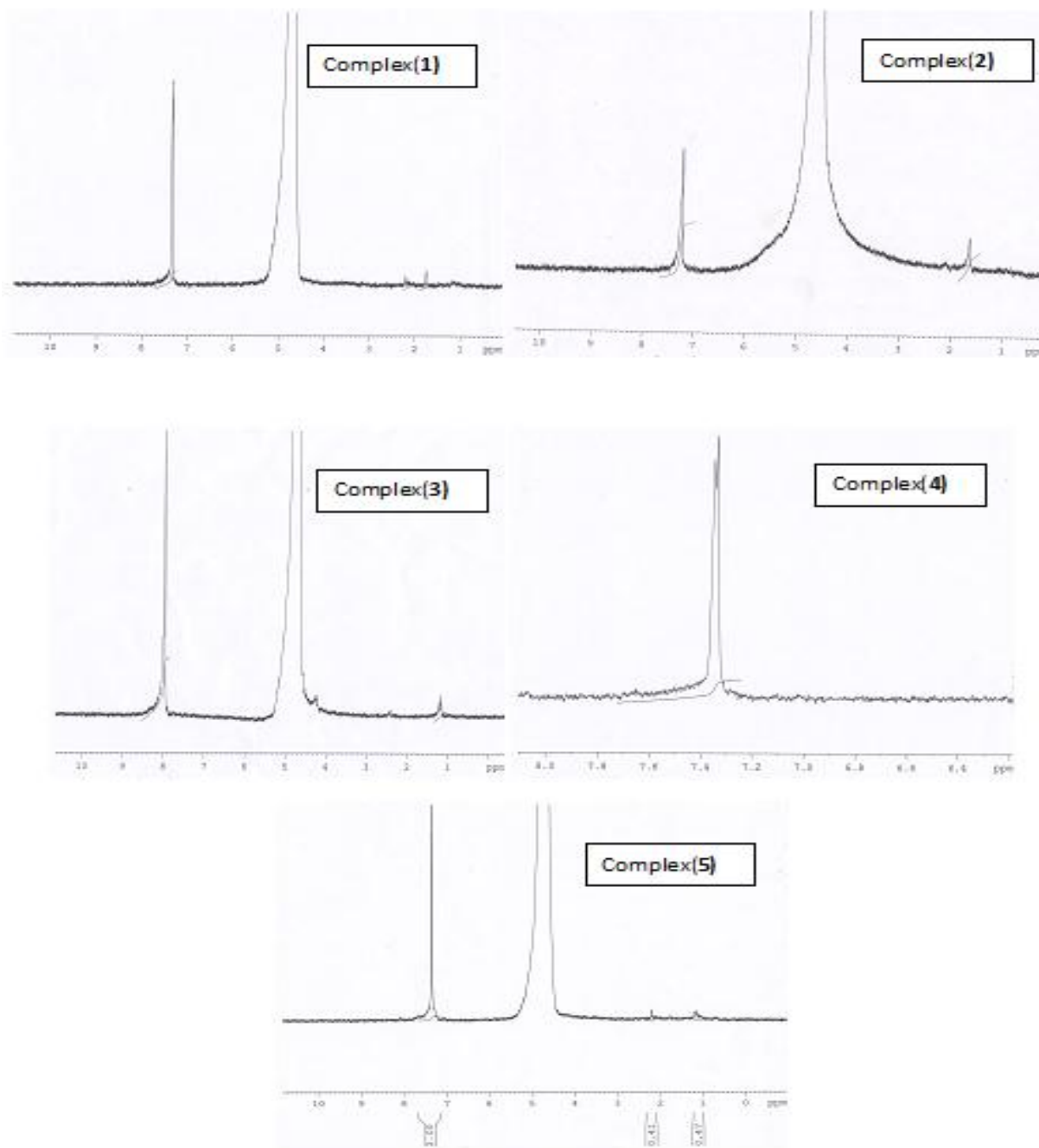
Table 1: FT-IR and UV-Vis data

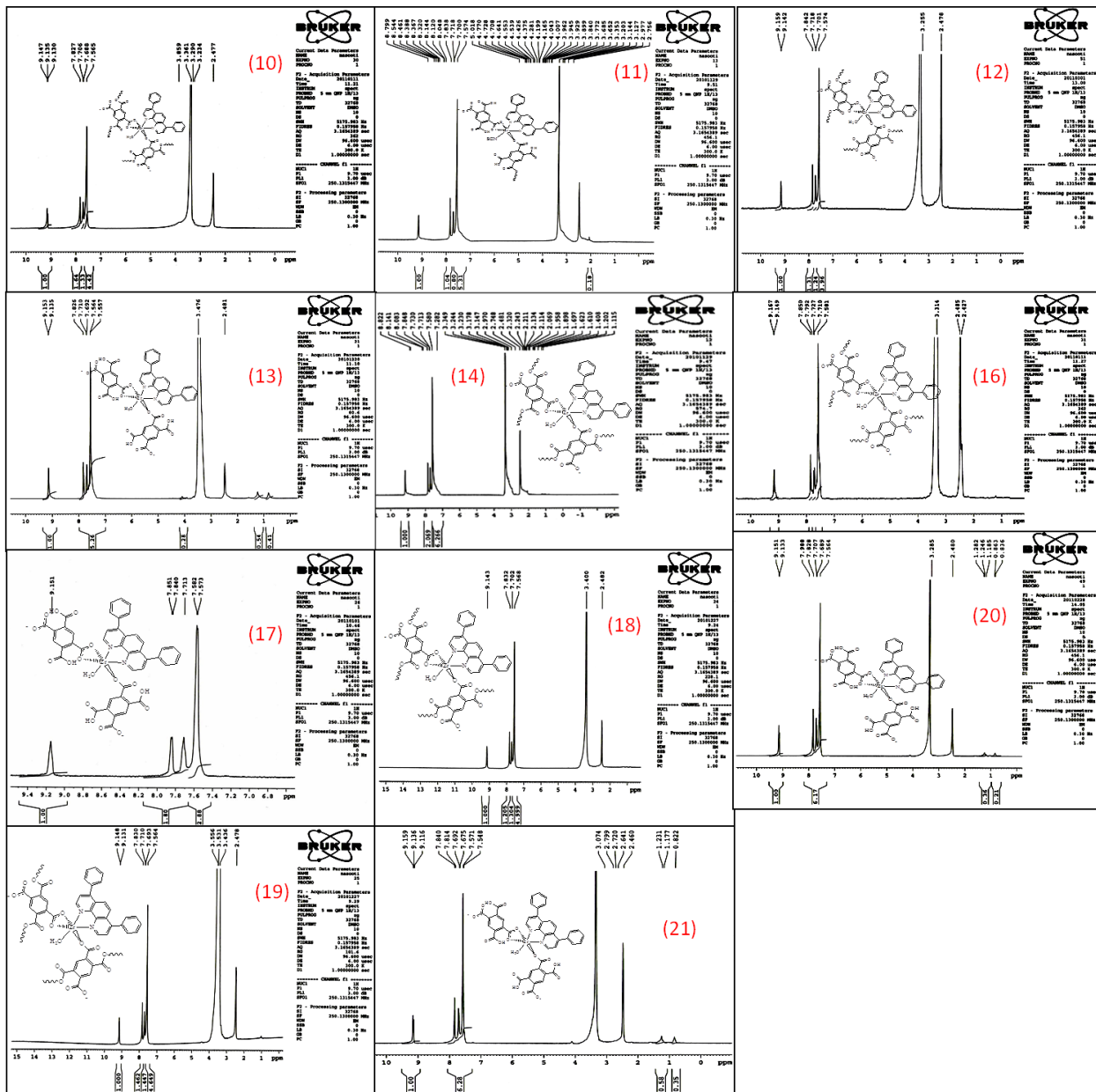
a:(cm⁻¹)

b: (nm)

IR ^a	IR ^a						UV-vis ^b	
	$\nu_{as}(\text{COO})$	$\nu_s(\text{COO})$	$\Delta\nu$	$\nu(\text{COOH})$	$\nu(\text{OH})$	$\nu(\text{C-N})$	$\Pi \rightarrow \Pi^*$	$n \rightarrow \Pi^*$
1	1554	1364	190				215 ,255	296
2	1545	1364	181				215 , 256	296
3	1505	1405	100	1711			215 , 255	297
4	1503	1438	65	1724			215 , 255	295
5	1551	1359	192				215 , 255	297
6	1551	1356	195				214 , 256	296
	1476	1317	159					
7	1611	1446	165	1706			214 , 255	295
	1509	1412	97					
8	1599	1378	221				207, 255	291
	1481	1416	65					
9	1577	1381	196				208, 255	291
	1482	1422	60					
10	1558	1374	184	—	3427	—	207 , 220 , 238,308 , 332	
	1487	1410	77				272	
11	1552	1378	174	—	3436	2061	206 , 219 , 238,308 , 332	
	1486	1410	76				272	
12	1552	1378	174	—	3434	—	205 , 220 , 238,308 , 331	
	1486	1410	76				274	
13	1552	1377	175	1722	3427	—	205 , 220 , 238,309 , 333	
	1485	1410	75				272	
14	1552	1378	174	—	3411	—	207 , 220 , 238,308 , 333	
	1484	1410	74				272	
15	1552	1377	175	1725	3444	—	204 , 220 , 238,309 , 332	
	1486	1411	75				273	
16	1551	1377	175	—	3402	—	205 , 220 , 238,308 , 331	
	1484	1410	75				272	
17	1552	1378	174	1719	3445	—	204 , 220 , 238,309 , 330	
	1486	1411	75				273	
18	1551	1378	173	—	3507	—	203 , 220 , 239,308 , 334	
	1484	1409	74				272	
19	1552	1378	174	1725	3434	—	204 , 220 , 238,310 , 331	
	1483	1410	73				272	
20	1551	1381	170	—	3462	—	203 , 220 , 238,309 , 334	
	1484	1410	74				273	
21	1551	1378	173	1725	3436	—	206 , 220 , 238,309 , 333	
	1484	1410	74				270	

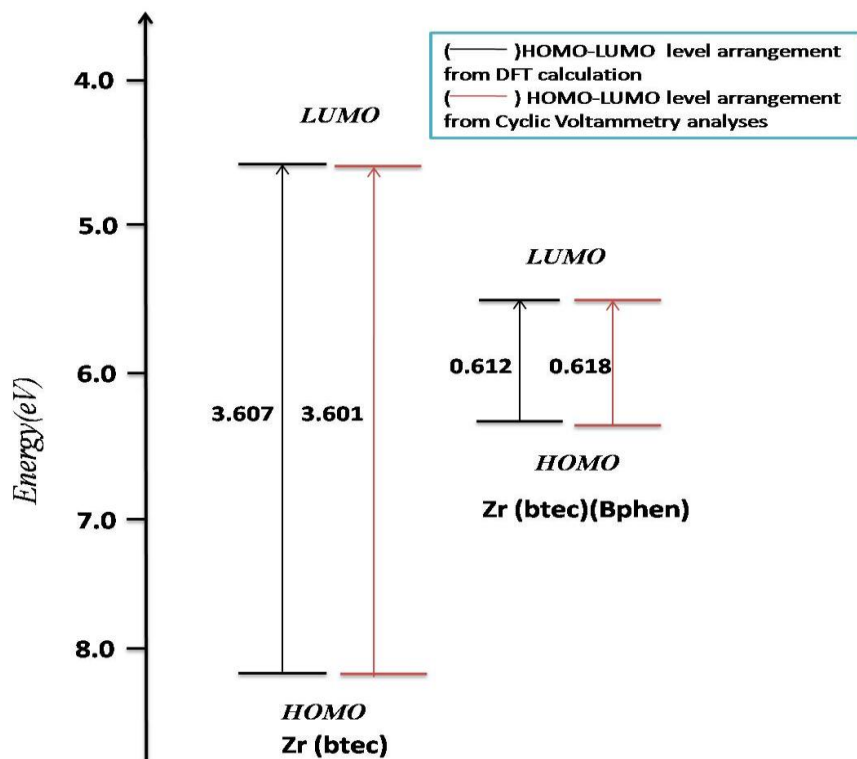
S2:NMR Spectra of Zr complexes recorded in DMSO solven at room temperature.





S3:

(-----) HOMO-LUMO level arrangement from DFT calculation and (-----) HOMO-LUMO level arrangement from Cyclic Voltammetry analyses.



S5:

HOMO-LUMO configuration for ligand to metal charge transfer (LMCT) in Zr(btec)(Bphen).

