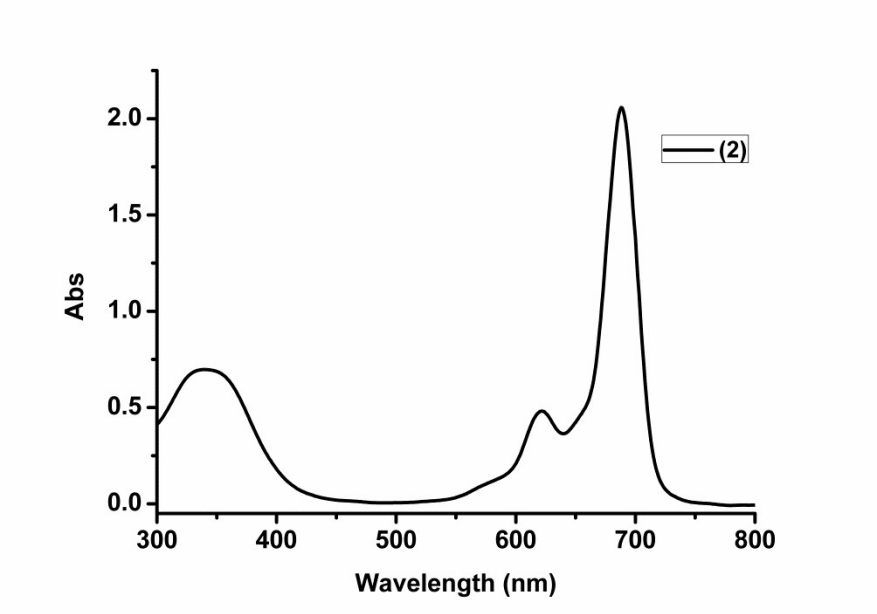

Fig. S1. UV-Vis spectra of the compound **(2)**

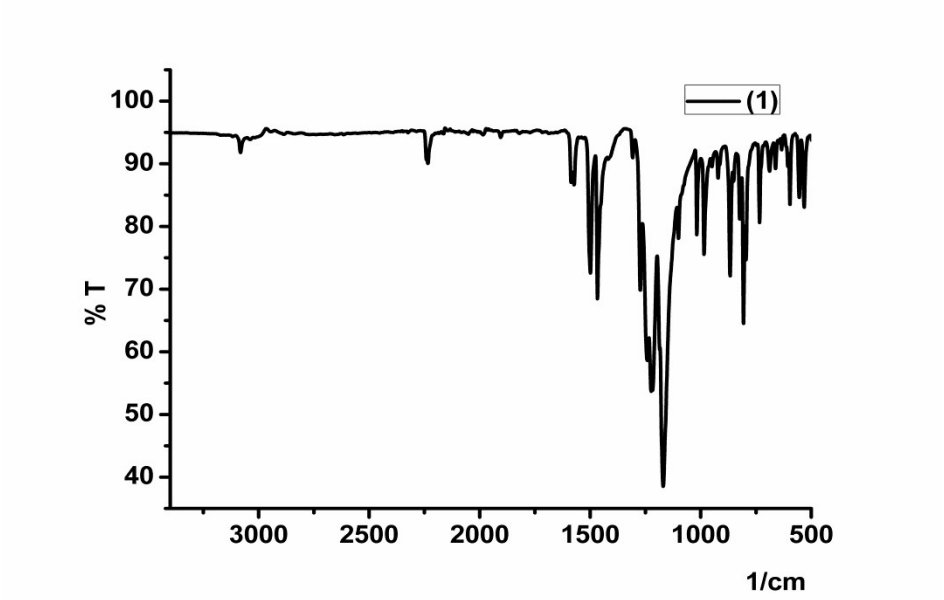

Fig. S2. FT-IR spectra of the compound **(1)**

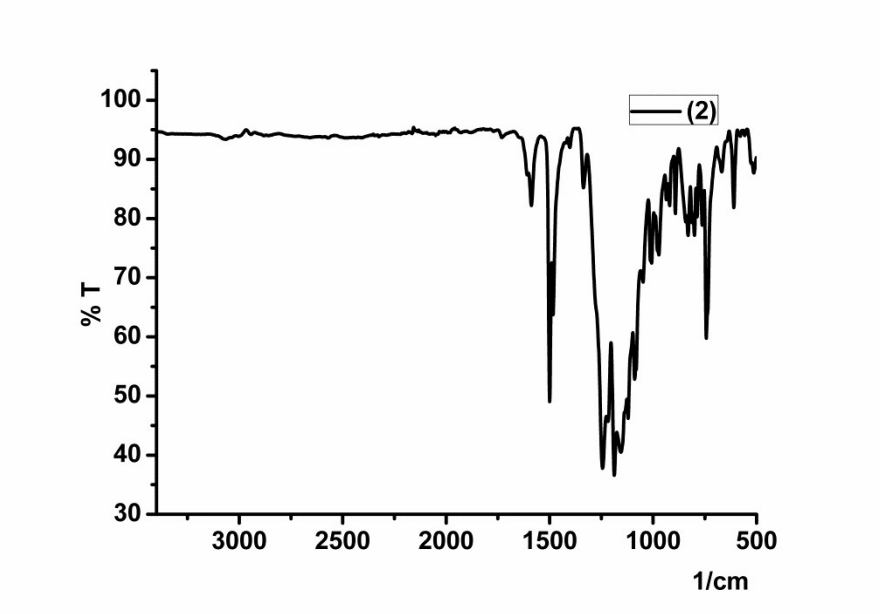

Fig. S3. FT-IR spectra of the compound **(2)**

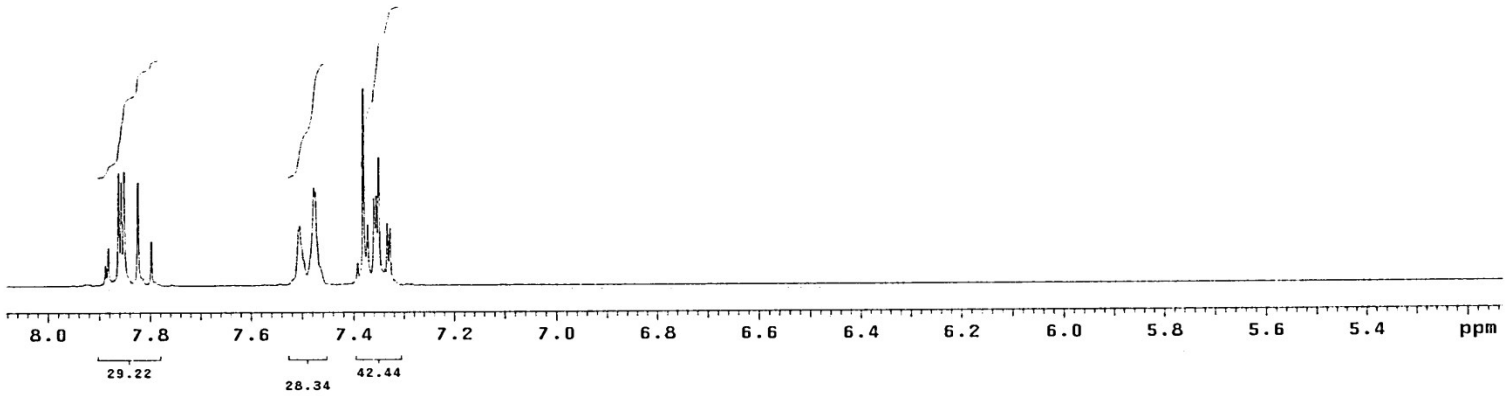

Fig. S4. ^{1}H-NMR spectra of the compound **(1)**

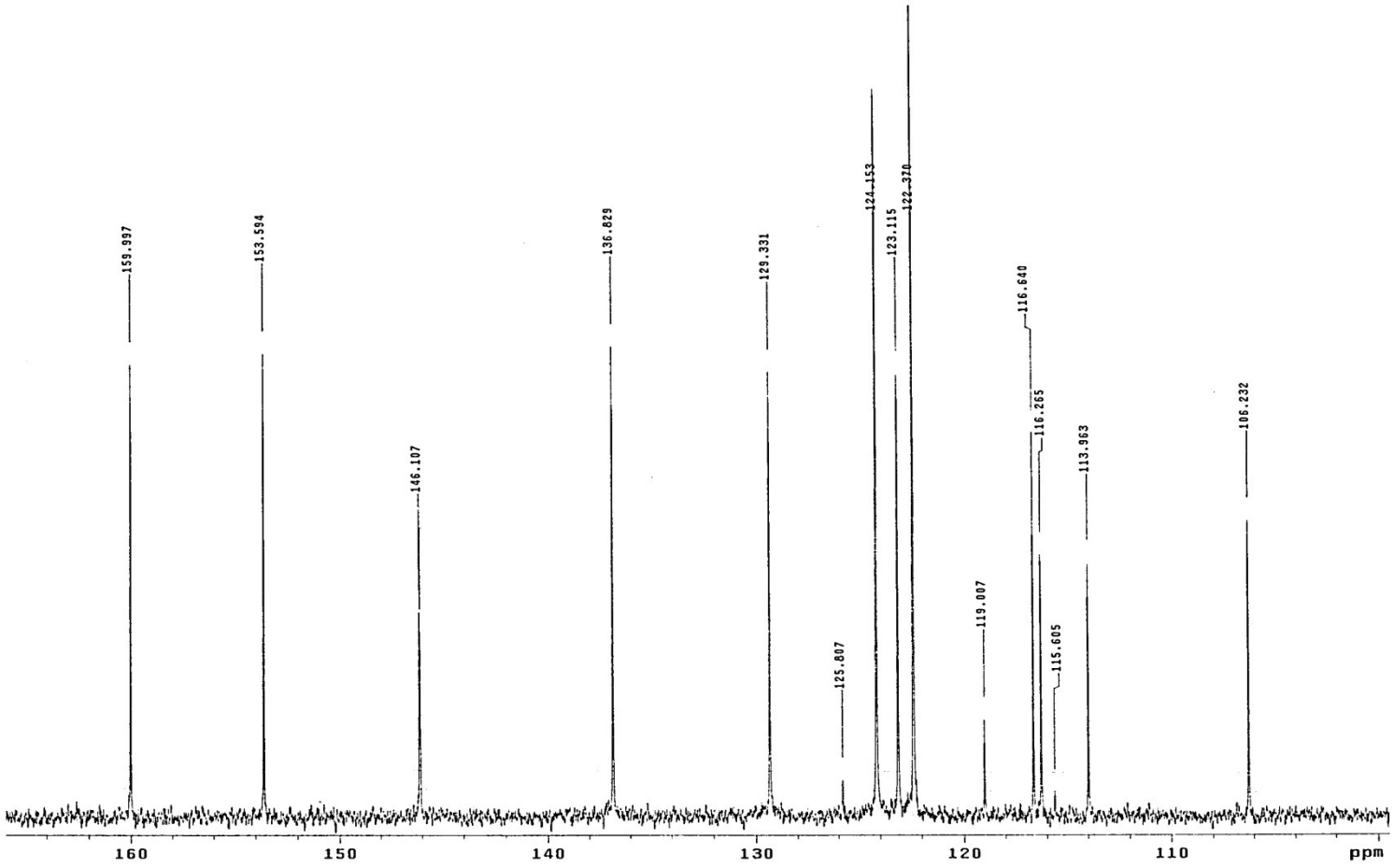

Fig. S5. ^{13}C-NMR spectra of the compound **(1)**

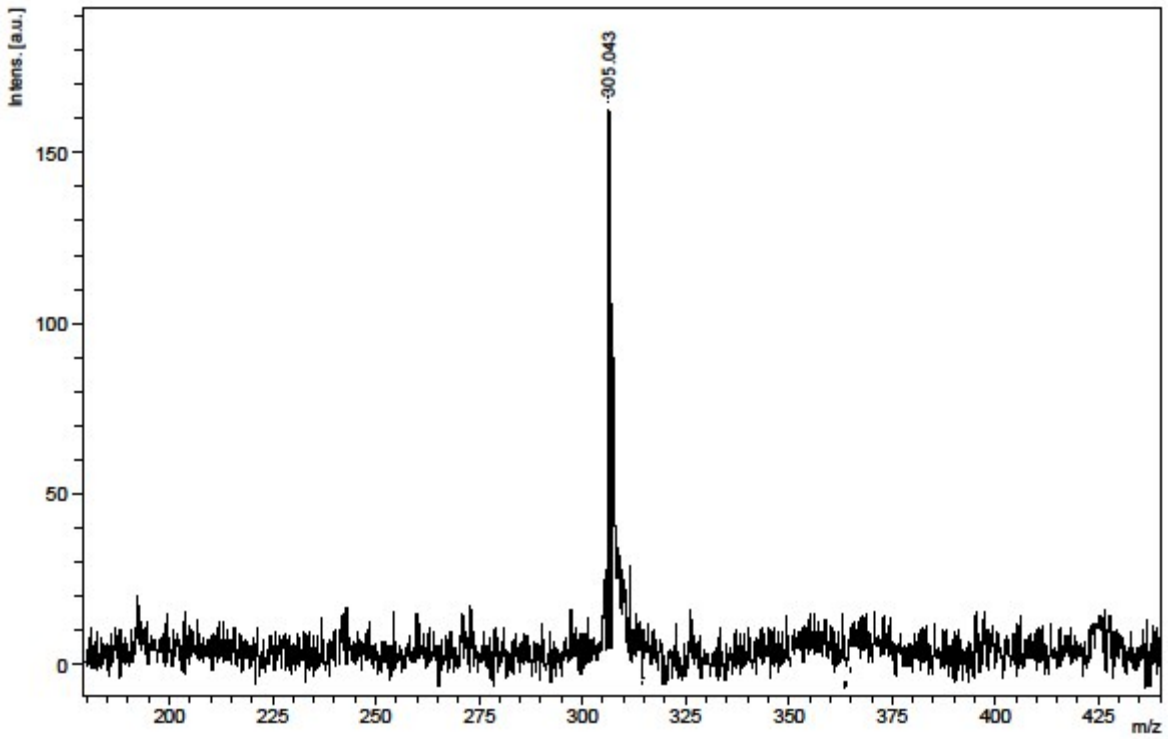

Fig. S6. MALDI-MS spectra of the compound **(1)**

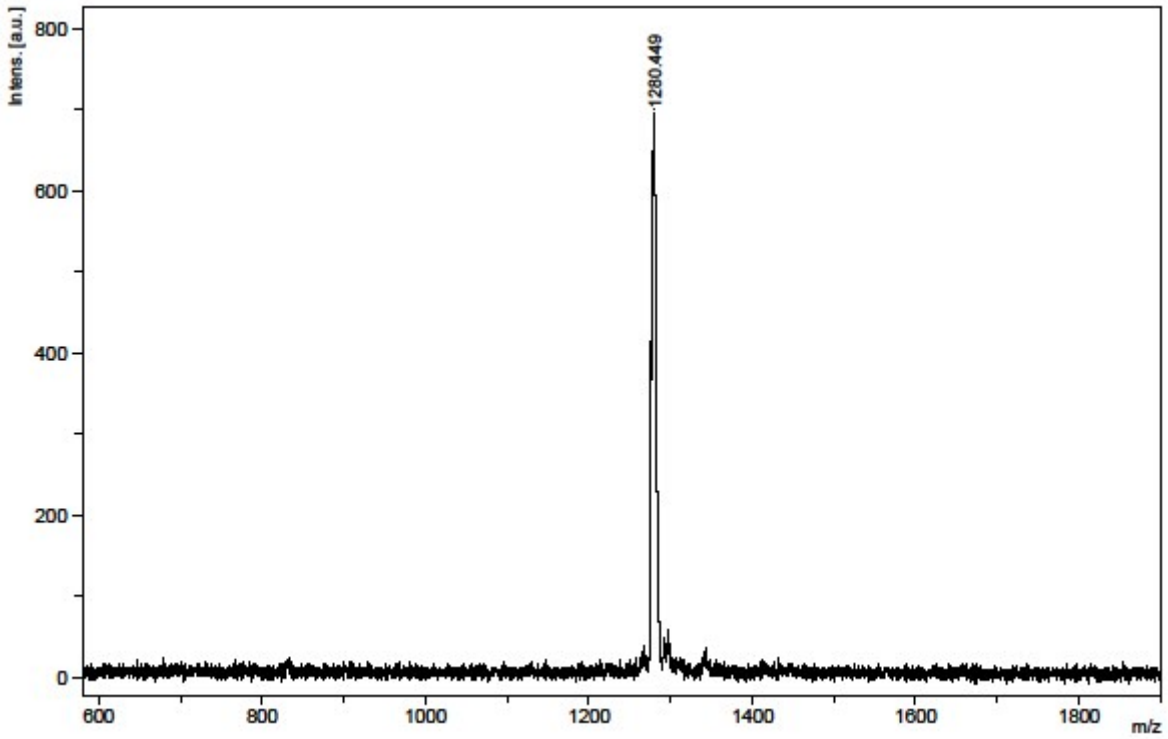

Fig. S7. MALDI-MS spectra of the compound **(2)**

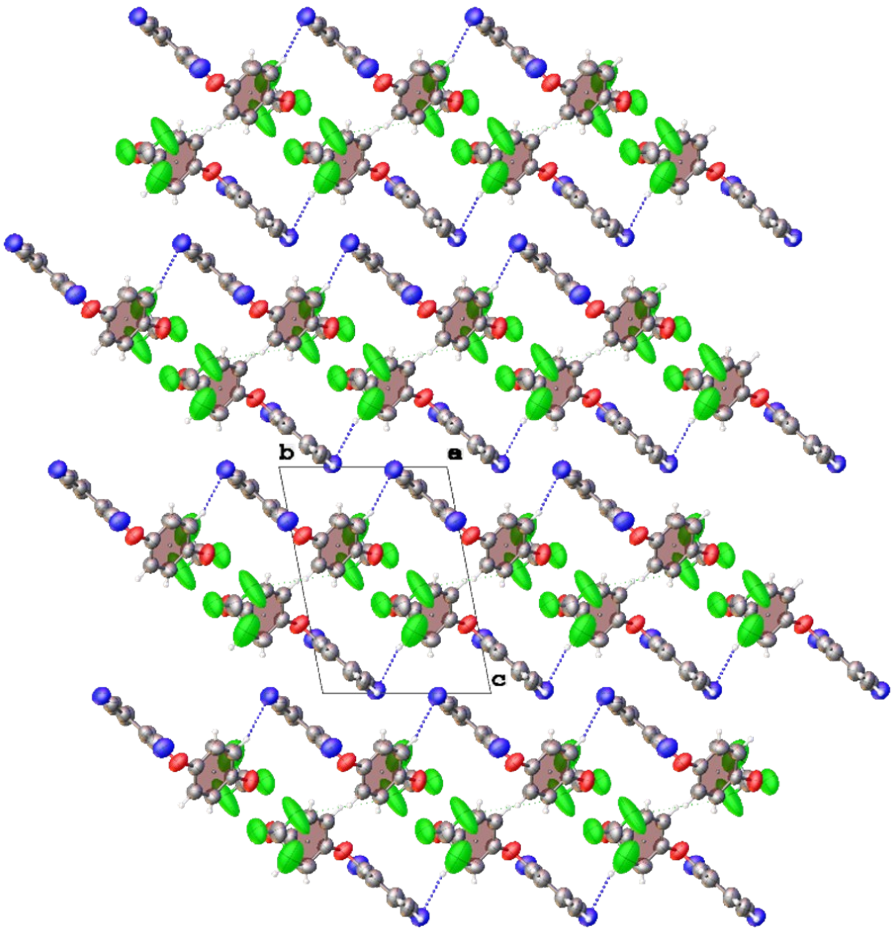

Fig. S8. The (100) view of the triclinic molecular assemblies of compound **(1)** with the stated unitcell. Blue dots indicate the C2—H2···N2 donor-acceptor interaction.

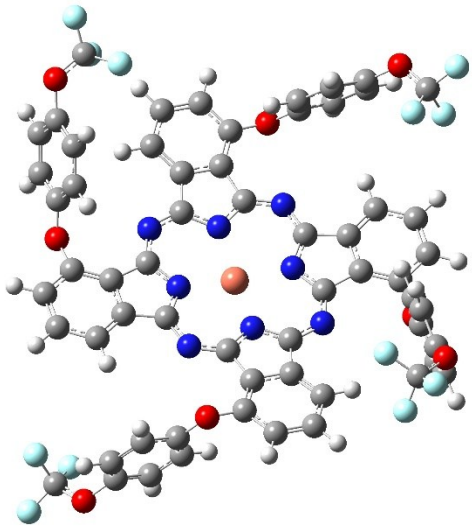

Fig. S9. Molecular structure of the obtained CuPc **(2)**

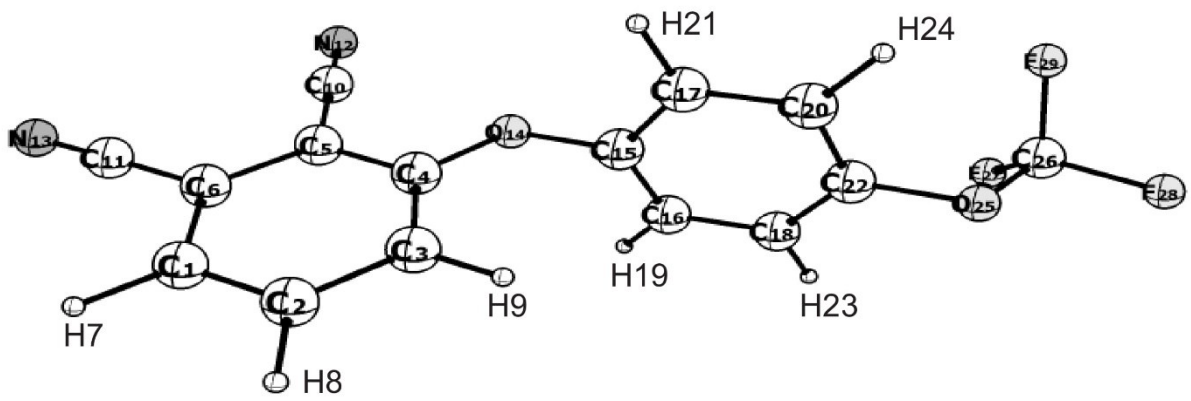

Fig. S10. Atomic labelling of the optimized structure of the compound **(1)**

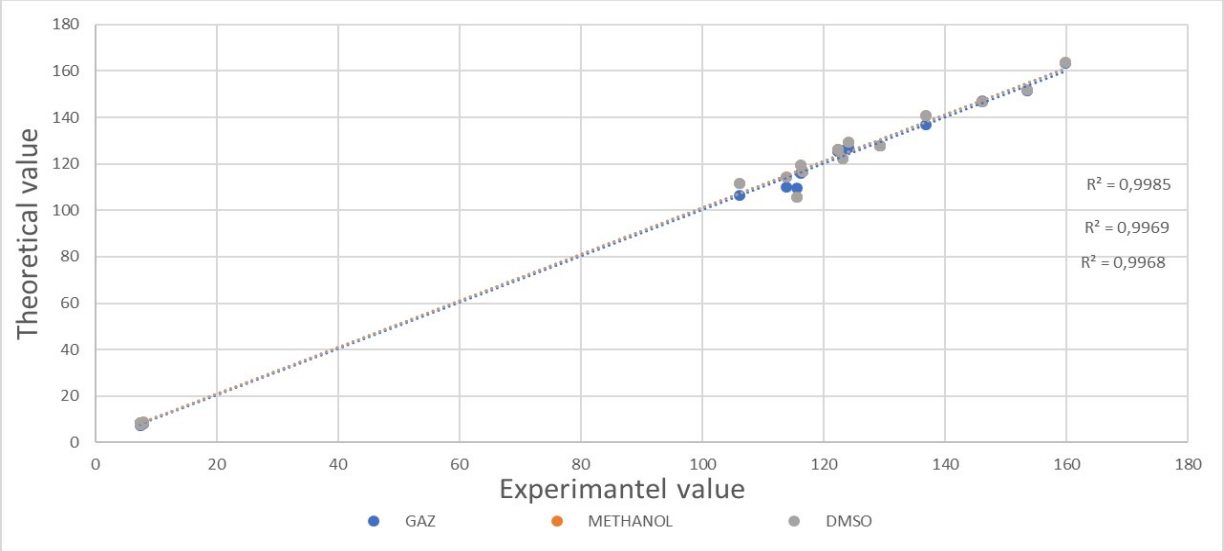

Fig. S11. Graph of experimental values against gas and DMSO phases in theorical calculations for the compound **(1)**

Fig. S12. IR spectrum of the compound **(1)**

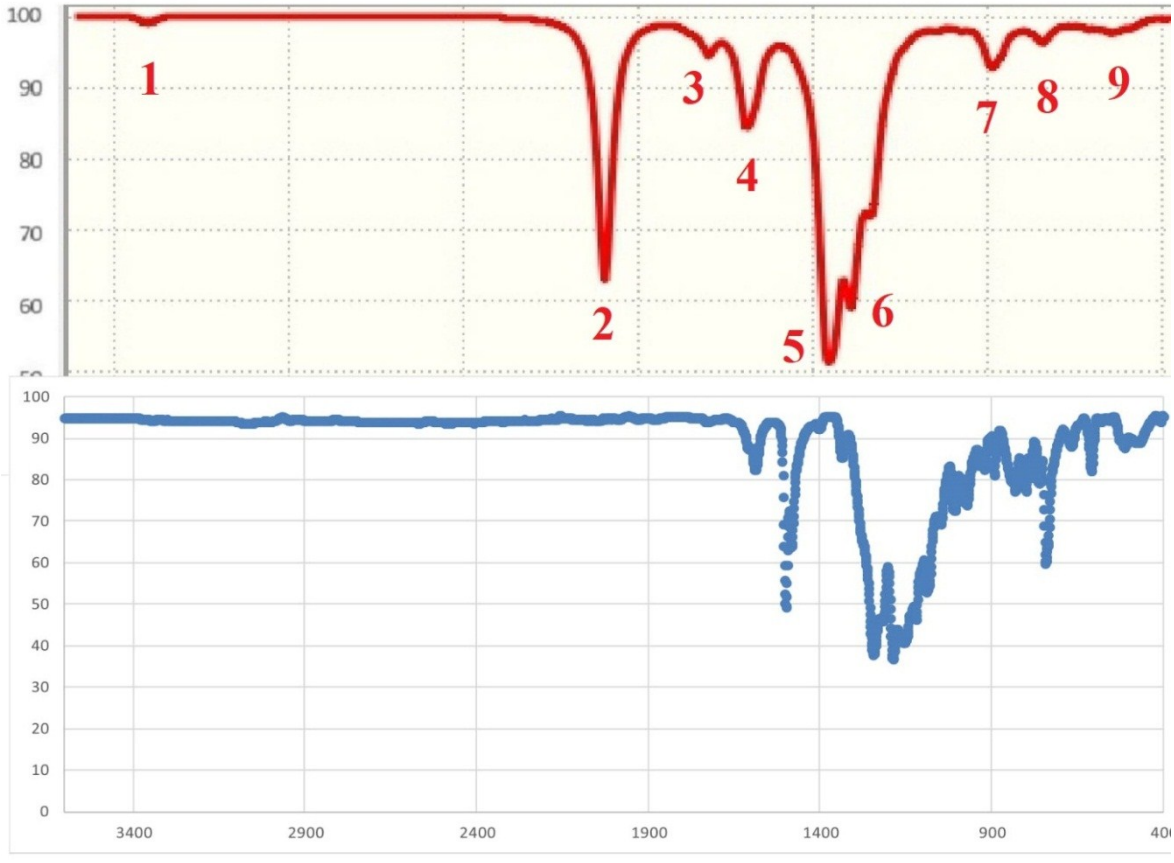

Fig. S13. IR spectrum of the CuPc **(2)**

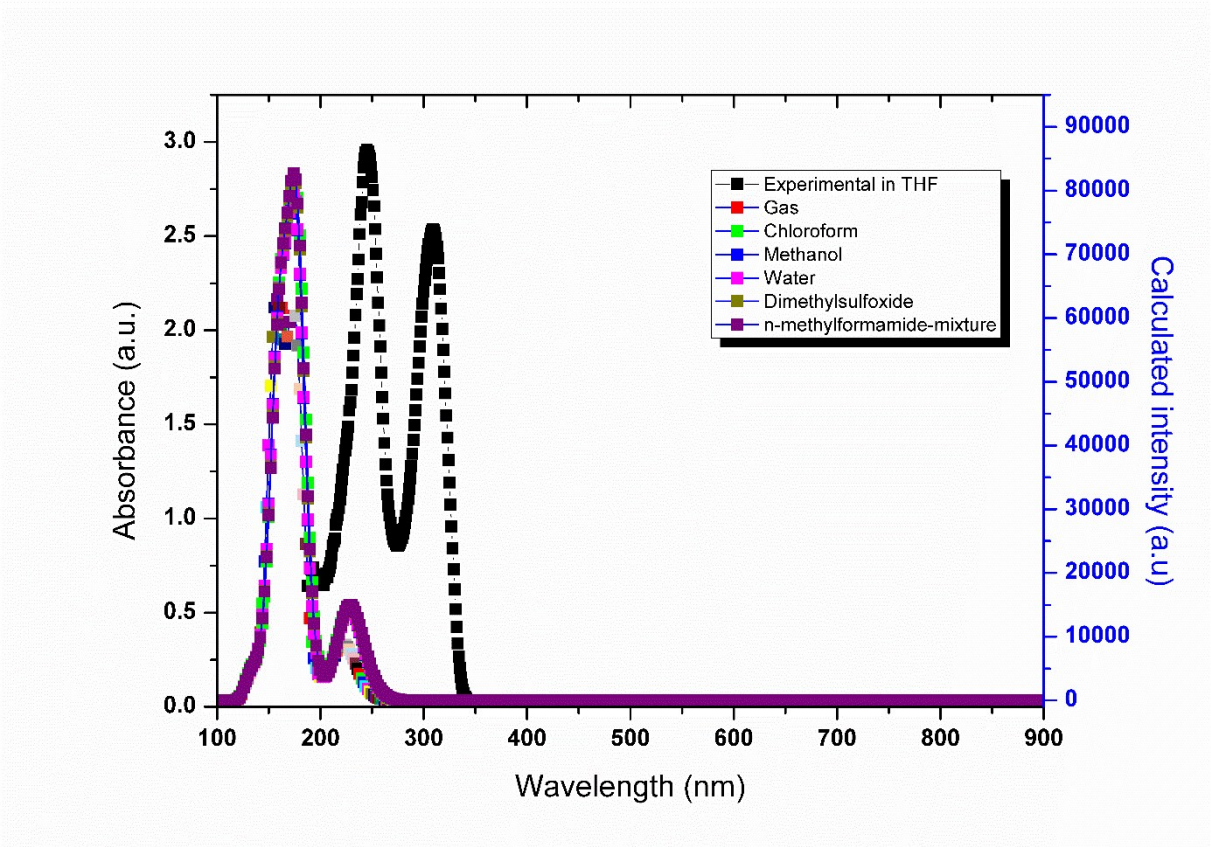

Fig. S14. UV-Vis spectrum of the compound **(1)**

Table S1. The possible inter-molecular π···π (*Cg*···*Cg*) interactions for the compound **(1)**. [a]

No	Cg(I) ···Cg(J)	Symmetry	Cg···Cg [b]	Cg(I)-perp [c]	Cg(J)-perp [d]	α [e]
1	Cg(1)···Cg(1)	-x, -y, 2-z	5.6354	3.5266	3.5266)	0.0
2	Cg(1)···Cg(1)	1-x, -y, 2-z	4.9619	3.4220	3.4220	0.0
3	Cg(1)···Cg(2)	x, -1+y, z	5.5629	3.5982	4.5937	82.499
4	Cg(1)···Cg(2)	1-x, -y, 2-z	5.8525	2.7042	4.4647	82.499
5	Cg(2)···Cg(2)	1-x, -y, 1-z	5.7802	2.9329	2.9329	0.0

[a] Cg···Cg < 6.0 Å. [b] Distances between centroids of the rings. [c] Perpendicular distance of Cg(I) on ring J plane (Å). [d] Perpendicular distance of Cg(J) on ring I plane (Å). [e] Dihedral angle between planes I and J (°).

Table S2. The possible inter-molecular Y—X···Cg interactions of the compound **(1)**. [a]

No	Y—X···Cg(I)	Symmetry	X···Cg(I) [b]	X-perp [c]	Y—X···Cg [d]	Y···Cg [e]
1	C(15)—F(2)···Cg(1)	1+x, 1+y, z	3.311	3.311	127	4.4513
2	C(15)—F(2)···Cg(2)	1-x, 1-y, 1-z	3.9718	3.675	99	4.3631
3	C(8)—N(2)···Cg(2)	-1+x, y, z	3.6804	3.659	156	4.7484

[a] X···Cg < 4.0 Å. [b] Distance between X atom and Cg (Å). [c] Perpendicular distance of X to ring plane (Å). [d] Angle between Y—X···Cg(I) (°). [e] Distance between Y and Cg(I) (Å).

Table S3. Energy value of metal atom in lanl2dz basis set

	B3LYP	HF	M062X
Cu^{2+}	-5308,47607	-5282,40567	-5309,81485

Table S4. Energy values of the molecules with different method (eV)

	(2)	**(ΔG)***
B3LYP/3-21g	-128218.2713	-34.2914
B3LYP/6-31g	-128860.7775	-34.2186
B3LYP/SDD	-128880.9754	-35.1349
HF/3-21g	-127508.5762	-28.9436
HF/6-31g	-128133.3988	-25.1109
HF/SDD	-128156.9054	-31.0708
M06-2X/3-21g	-128173.4899	-35.7542
M06-2X/6-31g	-128818.2923	-35.4677
M06-2X/SDD	-128840.2391	-36.1189

*using lanl2dz level for energy value of metal atoms

Table S5. Experimental and calculated ^{1}H-NMR and ^{13}C-NMR chemical shifts (ppm) of the compound **(1)**

	GAS	METHANOL	DMSO	EXP.
C1	127.05	129.43	129.47	124.1
C2	136.78	140.71	140.77	136.8
C3	115.91	119.42	119.47	116.2
C4	163.14	163.79	163.79	159.9
C5	109.49	105.51	105.45	115.6
C6	125.68	122.38	122.33	123.1
C10	106.46	111.53	111.59	106.2
C11	109.86	114.15	114.21	113.9
C15	151.6	151.67	151.67	153.6
C16	125.38	126.3	126.31	122.3
C17	125.39	126.31	126.32	122.3
C18	127.85	127.81	127.81	129.3
C20	127.85	127.81	127.81	129.3
C22	147.05	146.81	146.81	146.1
C26	116.65	116.78	116.79	116.6
H7	8.1	8.46	8.35	7.9
H8	8.28	8.77	8.77	7.9
H9	7.23	7.65	7.66	7.4
H19	8.11	8.34	8.35	7.75
H21	8.12	8.35	8.35	7.75
H23	8.44	8.59	8.59	7.41
H24	8.44	8.59	8.59	7.41

Table 5. Selected frequencies of the compounds **(1,2)** at HF/6-31G level

Compounds	**Band**	**Teo. Freq (cm^{-1})**	**Vibration Modes[a]**
Ligand (1)	1	3401	STRE (aromatic CH)
	2	2563	STRE (N≡C)
	3	1775	STRE (C-C)
	4	1689	BEND (H-C-C)
	5	1425	STRE (C-O)
	6	1077	TORS (H-C=C=C)
	7	1004	TORS (O-C=C=C)
	8	645	STRE (C-F)
CuPc (2)	1	3384	STRE (aromatic CH)
	2	2092	STRE (N-C)
	3	1792	STRE (C-C)
	4	1687	BEND (H-C-C)
	5	1455	STRE (C-O)
	6	1371	STRE (C-O)
	7	971	BEND (C-N-C)
	8	953	TORS (H-C=C=C)
	9	645	STRE (C-F)
	10	253	STRE (Cu-N)

11	223	BEND (Cu-N-C)
12	86	TORS (Cu-N-C-N)