Electronic Supplementary Information for: Synthesis, structure, characterization andphotophysical properties ofcopper(I) complexes containing polypyridyl ligands.

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Table S1

Experimental and theoretical IR spectral data of complexe**1** (cm^{-1}).

Assignment of the vibration	Experimental	Theoretical
ν_{N-H}	3168	3596
ν_{C-H}	3047	3056
ν_{C-H}	3012	3017
$\nu_{C=Nimine}$	1583	1551
$\nu_{C=Npyridine}$	1522	1519
$\nu_{C=C}$	1475	1481

Table S2

Experimental and theoretical IR spectral data of complexe**2** (cm^{-1}).

Assignment of the vibration	Experimental	Theoretical
ν_{C-H}	3057	3161
$\nu_{C=N}$	1584	1583
$\nu_{C=C}$	1476	1472

Table S3.

Experimental and theoretical values of selected bond lengths [Å] and bond angles [°] for the description of the coordination geometries of the copper (I) atoms in compounds **1** and **2**.

Compound 1		
Parameters	**Experimental value**	**Theoretical value**
Cu(1)-N(1)	2.023(3)	2.051
Cu(1)-N(3)	2.135(3)	2.190
Cu(1)-P(1)	2.248(10)	2.272
Cu(1)-P(2)	2.226(11)	2.251
N(1)-Cu(1)-N(3)	80.05(12)	78.28
N(1)-Cu(1)-P(2)	128.24(10)	126.03
N(3)-Cu(1)-P(2)	108.30(9)	109.75
N(1)-Cu(1)-P(1)	106.32(9)	106.16
N(3)-Cu(1)-P(1)	113.87(9)	113.12
P(2)-Cu(1)-P(1)	115.02(4)	117.19

Compound 2		
Parameters	**Experimental value**	**Theoretical value**
Cu(1)-N(1)	2.106(2)	2.169
Cu(1)-N(4)	2.137(2)	2.191
Cu(1)-P(1)	2.303(8)	2.299
Cu(1)-P(2)	2.260(8)	2.260
N(4)-Cu(1)-N(1)	78.22(9)	76.60
N(4)-Cu(1)-P(2)	113.55(7)	111.68
N(1)-Cu(1)-P(2)	125.95(6)	126.64
N(4)-Cu(1)-P(1)	97.87(7)	97.29
N(1)-Cu(1)-P(1)	99.93(6)	99.46
P(2)-Cu(1)-P(1)	127.66(3)	129.26

Table S4.
Geometrical parameters for the intermolecular hydrogen bonding interactions in the crystal structure of compound **1**(Å , °).

D-H···A	D-H	H···A	D···A	D-H···A
N2-H2′···O32^{i}	0.86	2.663	3.280(6)	130
N2-H2′···O33^{i}	0.86	1.995	2.845(5)	169
C7-H7···O32^{ii}	0.95	2.56	3.402(6)	148
C21-H21···O32^{i}	0.95	2.57	3.335(5)	138
C29-H29···O33^{ii}	0.95	2.63	3.460(5)	145
C39-H39···O31^{ii}	0.95	2.62	3.489(5)	151
C15-H15···N4^{iii}	0.95	2.62	3.357(5)	135

Symmetrycodes: (i) -x+1/2+1,+y-1/2,-z+1/2+1; (ii) x+1/2,-y+1/2,+z+1/2;(iii) -x+2,-y,-z+1

Table S5.
Geometrical parameters for the intermolecular hydrogen bonding interactions in the crystal structure of compound **2** (Å , °).

D-H···A	D-H	H···A	D···A	D-H···A
O4-H4B···O3	0.84	2.10	2.919(5)	164
O4-H4A···N3^{i}	0.84	2.64	3.262(3)	132
O4-H4A···N5^{i}	0.84	2.42	3.229(3)	160
C21-H21···O4	0.95	2.62	3.302(5)	129
C23-H23···O1^{ii}	0.95	2.38	3.312(3)	168
C40-H40···O3	0.95	2.45	3.301(4)	149
C53-H53···O1^{iii}	0.95	2.46	3.389(4)	164
C52-H52···N5^{iv}	0.95	2.68	3.315(4)	125

Symmetrycodes: (i) x,+y+1,+z; (ii) x-1,+y,+z; (iii) x,+y-1,+z;(iv) x+1,+y,+z

Table S6.

Electronic excited states, calculated by time dependent density functional theory (TD-DFT) at M06/DZVP+6-31g(d) level of calculation.

Complex	E [nm] (eV)	Oscillator Strength	Transition (CI coef.)	Assignment
1	424.5 (2.92)	0.0701	HOMO→LUMO (0.98)	MLCT/XLCT/LLCT
	306.5 (4.05)	0.0188	HOMO-4→LUMO (0.85)	LLCT
	285.0 (4.35)	0.0422	HOMO→LUMO+6 (0.45) HOMO→LUMO+2 (0.21)	MLCT/XLCT/LLCT MLCT/XLCT/LLCT
	275.5 (4.50)	0.0363	HOMO→LUMO+7 (0.48)	MLCT/XLCT/LLCT
2	**E [nm] (eV)**	**Oscillator Strength**	**Transition (CI coef.)**	**Assignment**
	461.1 (2.69)	0.0387	HOMO→LUMO (0.80)	MLCT/XLCT/LLCT
	444.1 (2.79)	0.0238	HOMO→LUMO+1 (0.79)	MLCT/XLCT/LLCT
	431.5 (2.87)	0.0170	HOMO-1→LUMO (0.83)	MLCT/LLCT
	313.4 (3.96)	0.0047	HOMO-4→LUMO (0.50)	LLCT

* Metal-to-ligand charge transfer (MLCT)
* Ligand-to-ligand charge-transfer (LLCT)
* Phosphine-to-ligand charge transfer (XLCT)

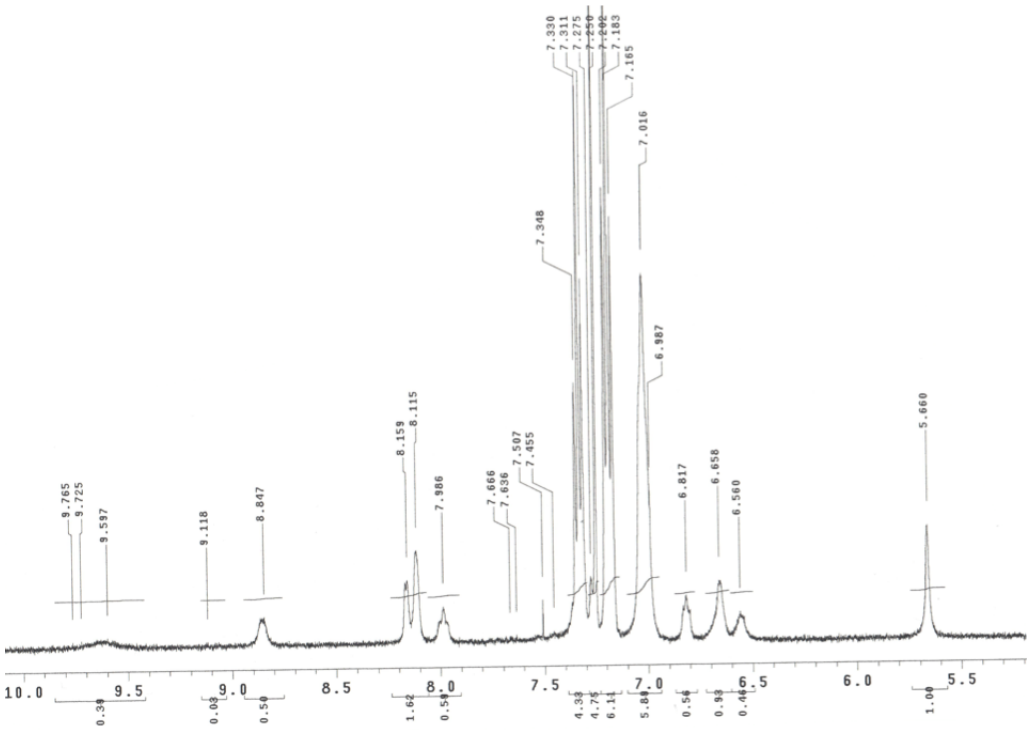

Figure S1. [1]H NMR spectrum of **1**.

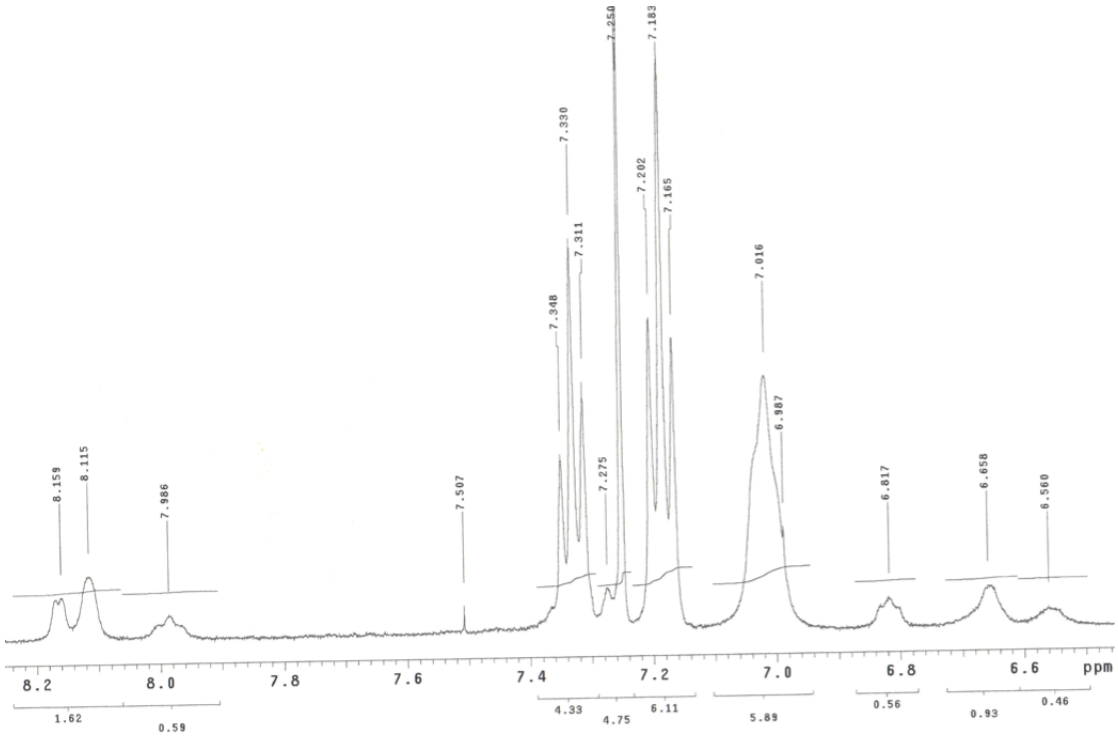

Figure S2. Partial [1]H NMR spectrum of **1**.

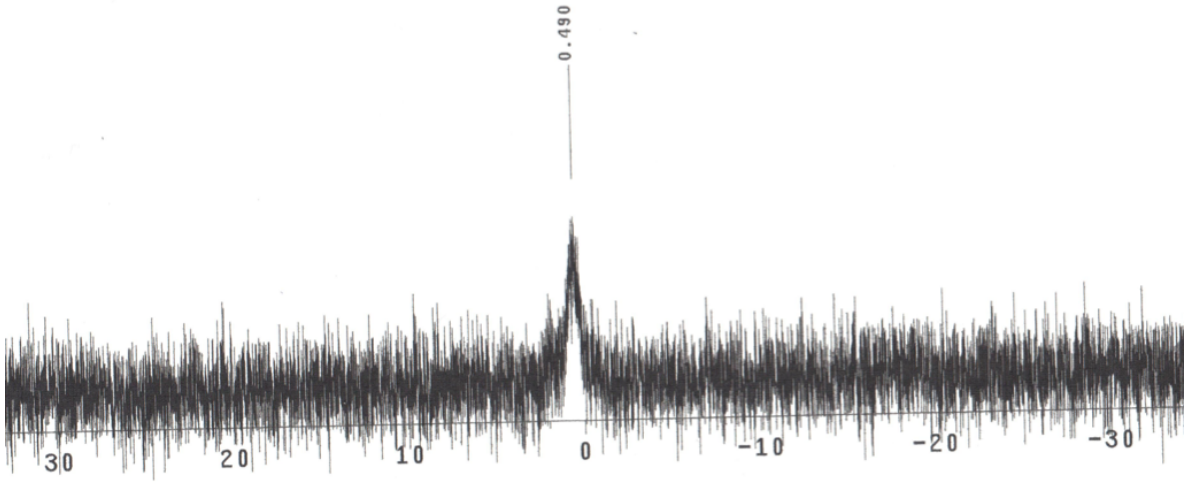

Figure S3. ^{13}P $\{^{1}H\}$ NMR spectrum of **1**.

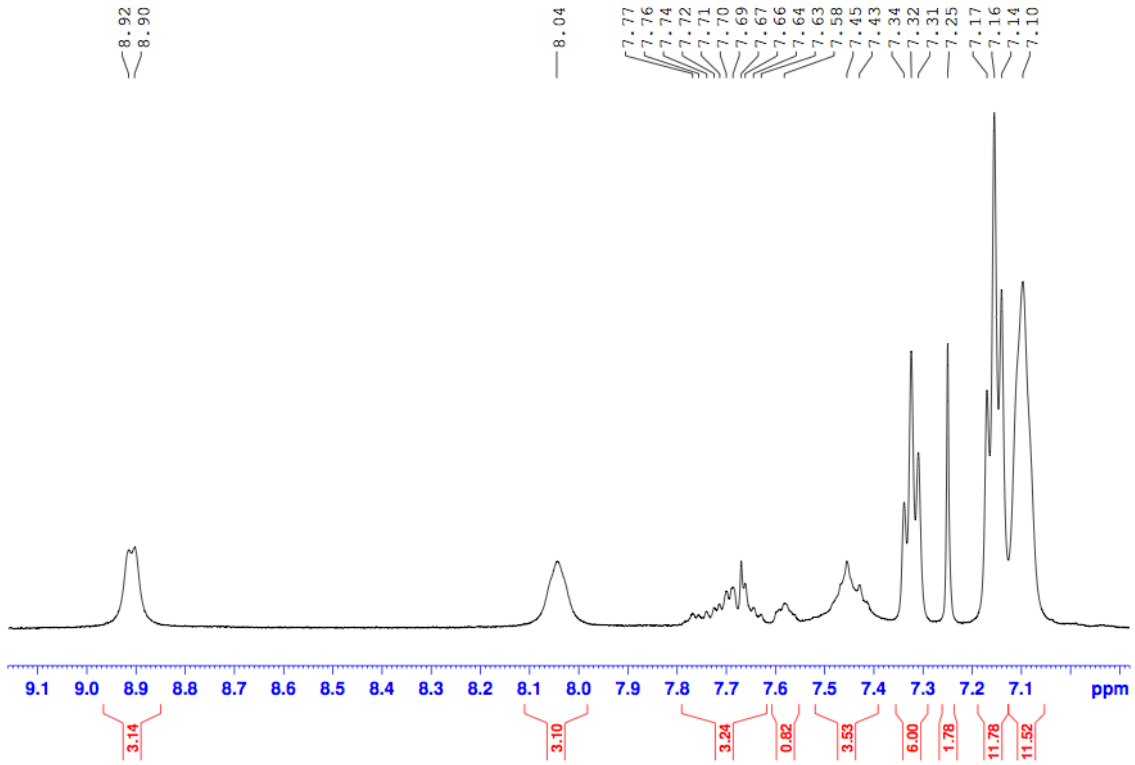

Figure S4. ^{1}H NMR spectrum of **2**.

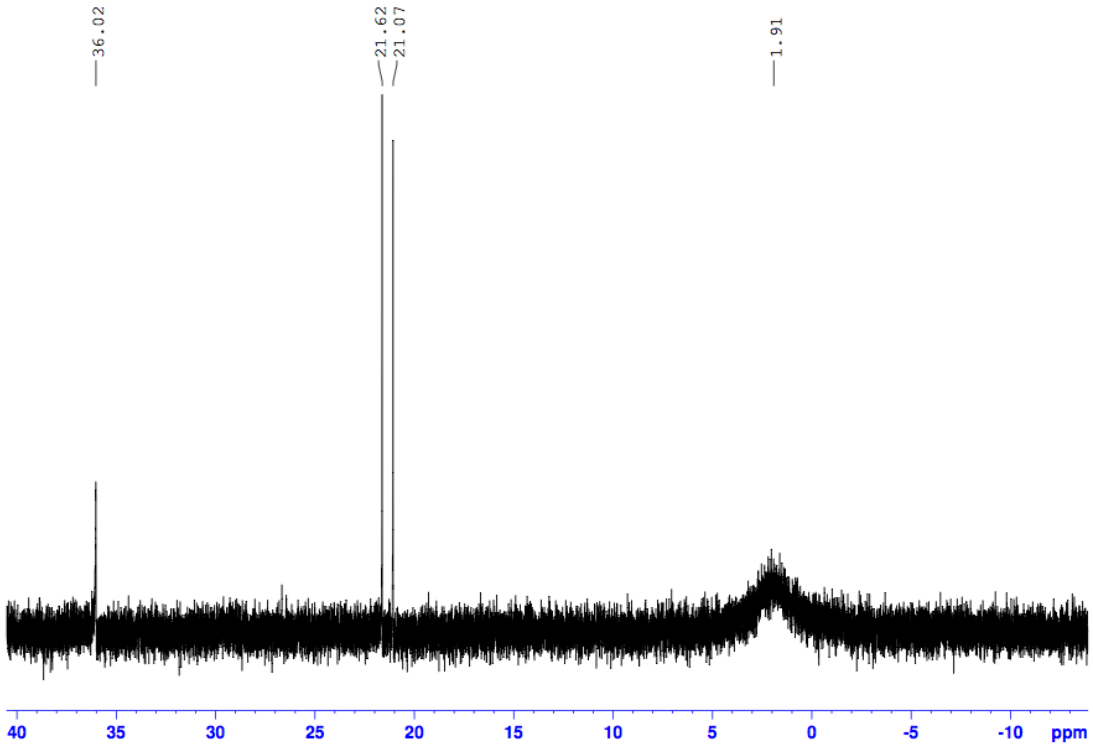

Figure S5. ^{31}P $\{^{1}H\}$ NMR spectrum of **2**.

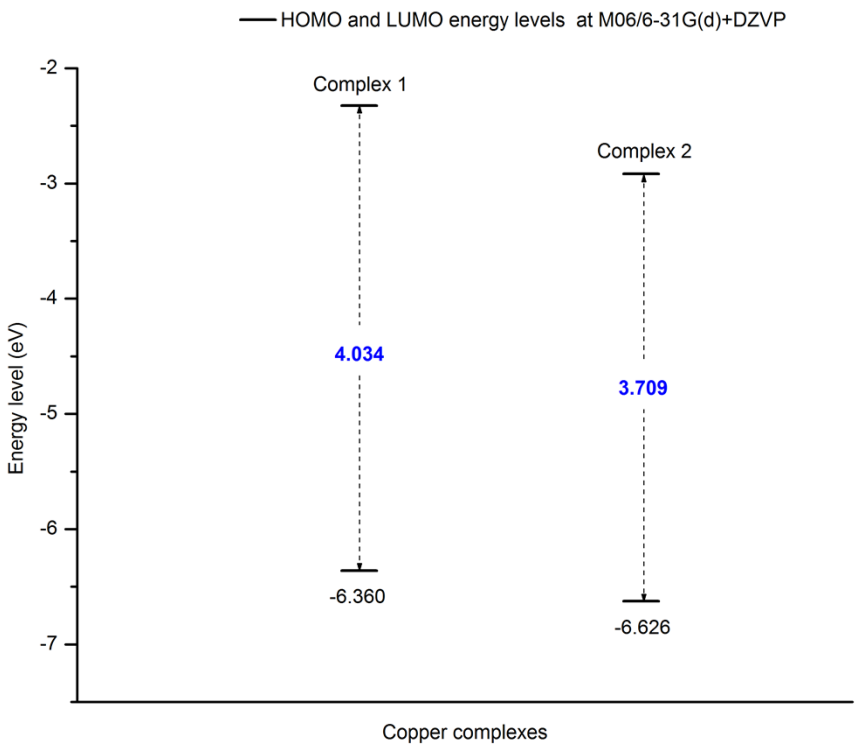

Figure S6. Molecular orbitals energy levels (HOMO and LUMO) with the M06/6-31G(d)+DZVP level of calculation.

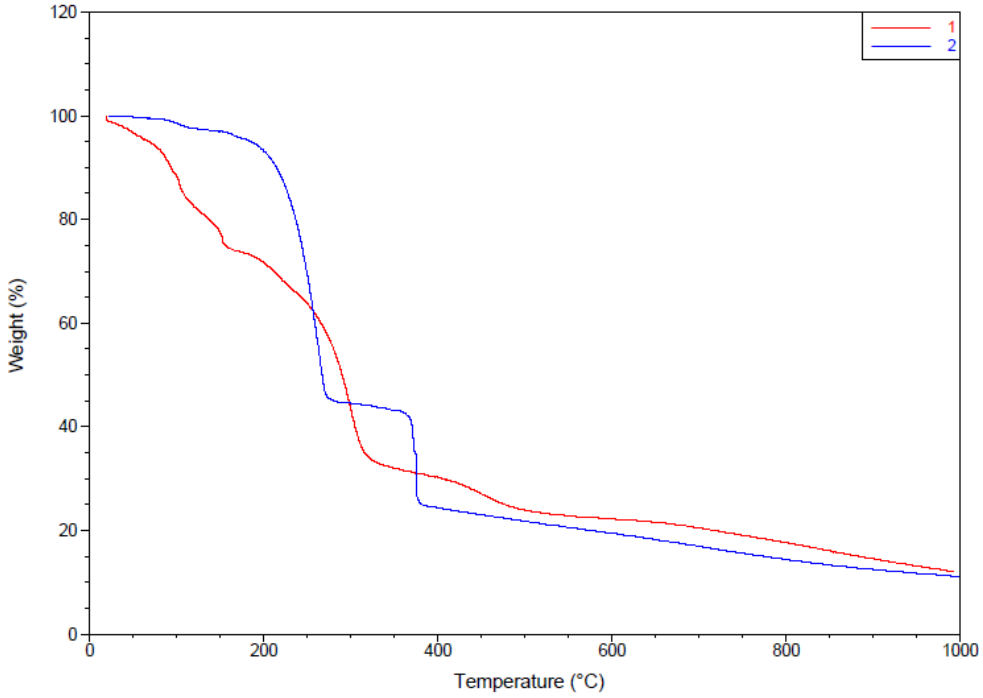

Figure S7. Thermograms of compounds **1** and **2**.