Supporting Information for

Synthesis of novel pyridyl containing phospholanes and their luminescent polynuclear copper(I) complexes

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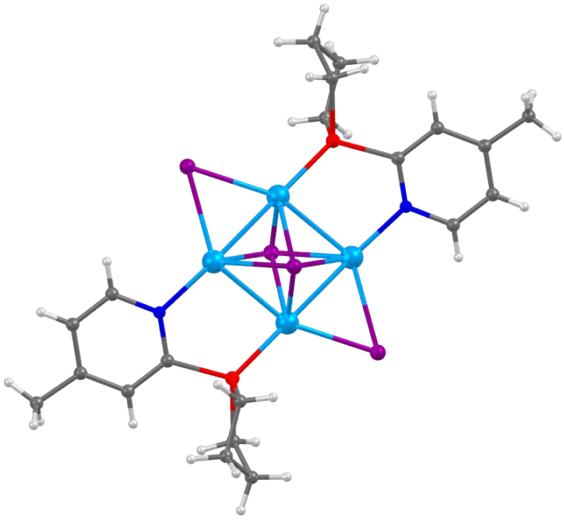
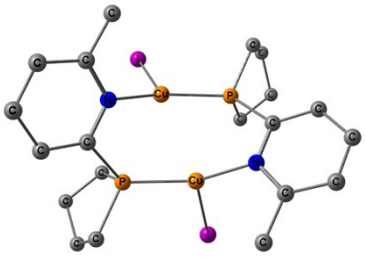
Contents

Figure S1 Molecular structure of complex **13***.



Colour legend: copper, light blue; nitrogen, blue; phosphorous, red; iodine, plum; carbon, grey; hydrogen, light grey.

Figure S2 Ground-state structure of complex **14**, optimized at PBE0-D3/def-TZVP level.



***** Picture was generated with DIAMOND Version 3.2k (Copyright Crystal Impact GbR)

Table S1. Cartesian coordinates of the ground-state structure of complex **14**, optimized at PBE0-D3/def-TZVP level**.**

	X	Y	Z
I	-2.912116794	1.372694119	-2.095563944
I	2.913161340	-1.373166896	-2.093801756
Cu	-1.302598769	0.611329494	-0.213858725
Cu	1.302652081	-0.611392869	-0.213105405
P	0.296773398	2.155383533	-0.394070732
P	-0.296641847	-2.155473571	-0.393814239
N	-2.165013312	-0.815971299	0.912633756
N	2.164493671	0.816140215	0.913535262
C	-1.763374840	-2.084207490	0.718543911
C	-2.421280810	-3.152248255	1.305936035
C	-3.519809673	-2.894777980	2.111598716
C	-3.928150740	-1.586699955	2.300224596
C	-3.234996610	-0.555019457	1.678065740
C	-3.628411212	0.873406641	1.818821570
C	1.762934308	2.084340070	0.719041387
C	2.420460849	3.152472648	1.306689718
C	3.518846287	2.895177281	2.112605738
C	3.926822714	1.587100676	2.302020705
C	3.234202592	0.555338890	1.679403845
C	3.628394747	-0.872943249	1.819451622
H	-2.092303257	-4.167646398	1.130751070
H	-4.055597966	-3.710146568	2.584420049
H	-4.781226058	-1.353673116	2.925103811
H	-2.780232842	1.463633717	2.177422582
H	-4.462523355	0.994208833	2.509355685
H	-3.906910276	1.273296356	0.837688960
H	2.091033876	4.167786792	1.131867184
H	4.055130224	3.710711433	2.584575756
H	4.778892046	1.354099159	2.928279616
H	4.462390797	-0.993664023	2.510139682
H	3.907381771	-1.272124241	0.838166174
H	2.780453742	-1.463850373	2.177493989
C	1.301524129	3.792127687	-2.267622373
C	0.043303277	4.488799162	-1.760494100
C	1.086035911	2.298532940	-2.065407351
C	-0.301901877	3.915614505	-0.380790771
H	2.177427227	4.124846379	-1.699628244
H	0.352790761	1.903453394	-2.773269125
H	-0.783588636	4.271093325	-2.441753555
H	-1.376132954	3.910629199	-0.197014879
H	0.161059728	5.574352994	-1.717456550
H	0.177542088	4.464509636	0.431772220
H	1.983991606	1.682331272	-2.127229757
H	1.492822529	4.021243520	-3.318947362
C	-1.085041351	-2.298906496	-2.065547775
C	-1.300854253	-3.792526316	-2.267282924
C	0.302027952	-3.915691168	-0.379976995
C	-0.042892844	-4.489244269	-1.759574972
H	-0.351292052	-1.904322919	-2.773159032
H	-2.176966353	-4.124843476	-1.699373264
H	-0.177602682	-4.464391655	0.432606250
H	1.376220088	-3.910647352	-0.195968349
H	-0.160822372	-5.574766440	-1.716217143
H	0.784227131	-4.271883749	-2.440671246
H	-1.491945715	-4.021980539	-3.318570111
H	-1.982767417	-1.682443748	-2.128044950

Figure S3 Calculated (dashed lines) and experimental (solid line) absorption spectra of compound **4**. Experimental bands at 281 and 255 nm correspond to computed lines at 261, 251, 248 and 235 nm. Main contributions arise from transitions between HOMO-1, HOMO and LUMO, LUMO+1, depicted at Figure S4. The HOMO is localized on both the π orbitals of pyridyl moiety and the lone pair of P atom. HOMO-1 involves both the π orbitals of pyridyl moiety and the lone pair of N atom. LUMO and LUMO+1 are localised mainly on π* orbitals of pyridyl moiety. Thus, the experimetal bands should be assigned to transitions of mixed n–π* and π–π* character.

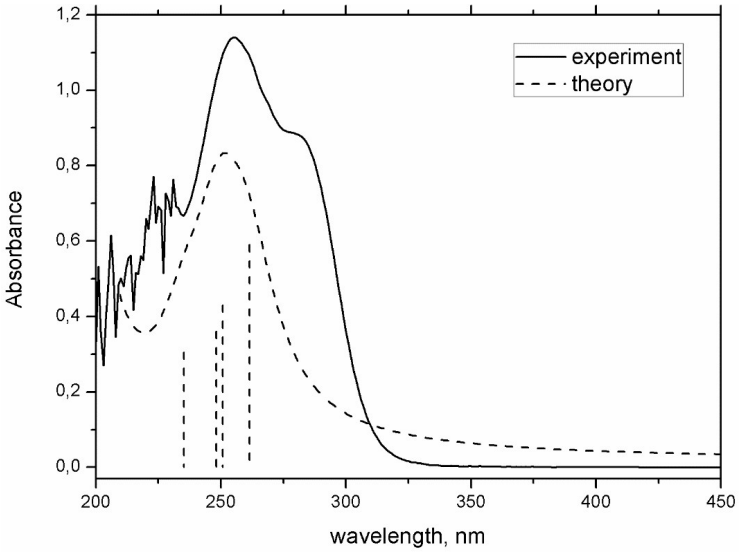
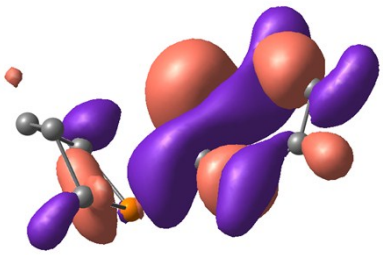
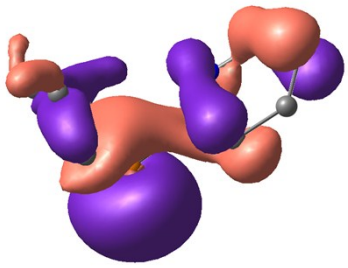


Figure S4 Frontier orbitals of **4**.

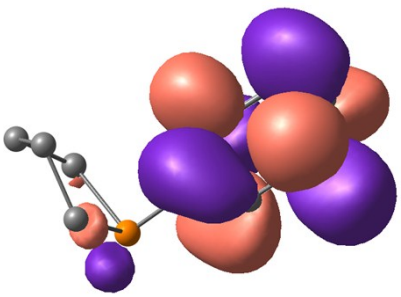
HOMO-1



HOMO



LUMO



LUMO+1

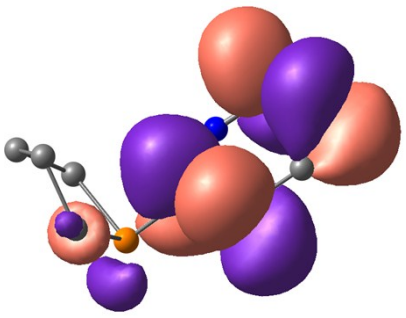


Figure S5 Calculated absorption spectra of compounds **4** and **10-14**.

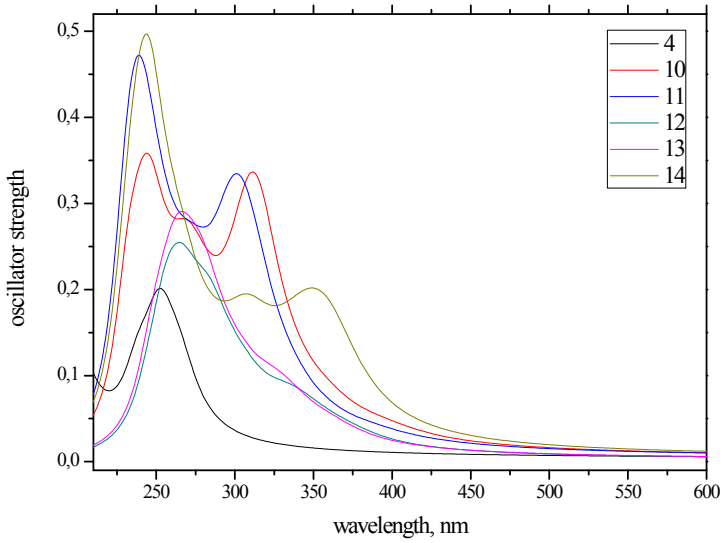


Figure S6 Schematic representation of the molecular orbitals for the singlet ground state of **12**.

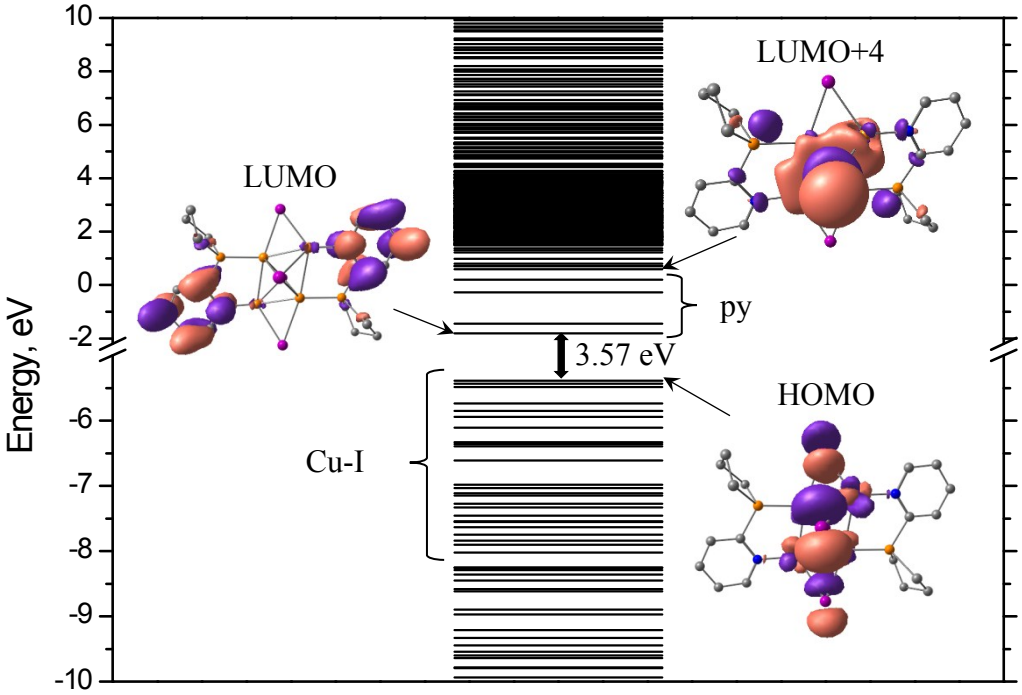


Figure S7 ORTEP drawing of the molecular structure of complex **10**[*]**.** Hydrogen atoms are omitted for clarity.

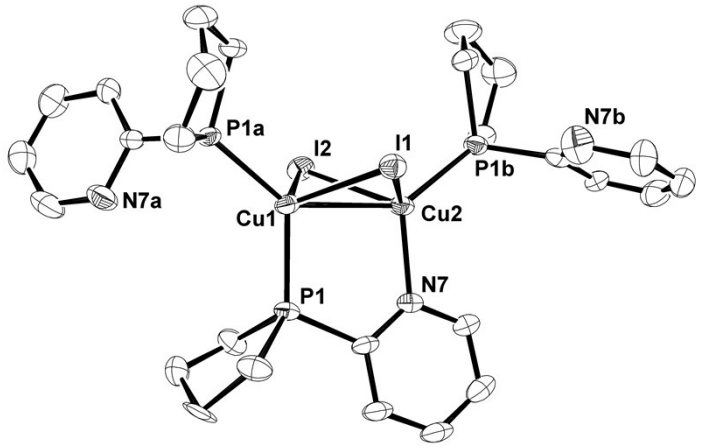
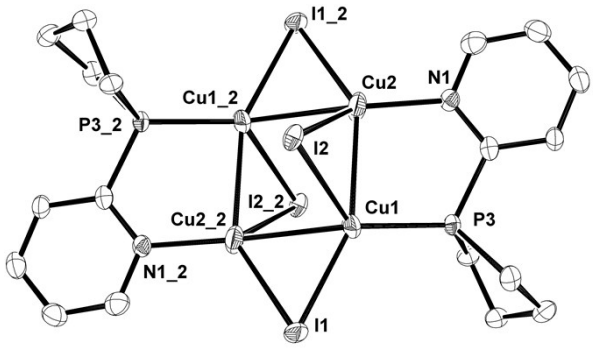


Figure S8 ORTEP drawing of the molecular structure of complex **12**[*]**.** Hydrogen atoms are omitted for clarity.



[*]Pictures were generated with ORTEP3 for Windows[1]

[1] Sheldrick, G.M. A short history of SHELX SHELX (2008). Acta Cryst. A64, 112-122