Electronic supporting information

Cu(I) and Pb(II) complexes containing new tris(7-naphthyridyl)methane derivatives: Synthesis, structures, spectroscopy and geometric conversion

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Figure S1. The absorption spectra of $\mathbf{L^1}$ in CH_2Cl_2 (solid line), CH_3CN (dashed line) and CH_3OH (dashed dot line).

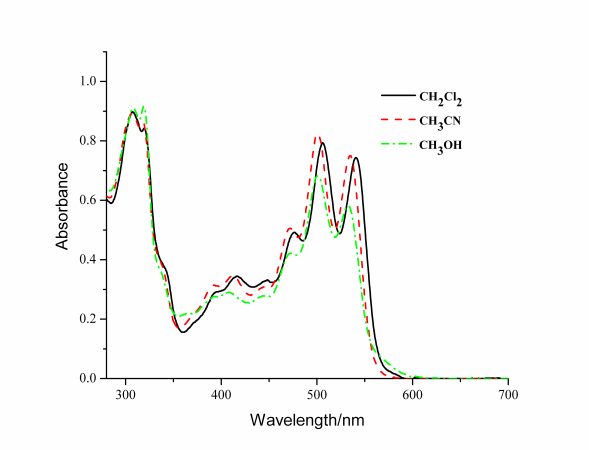


Figure S2. Plots of the relevant HOMO and LUMO for $\mathbf{L^1}$ and. $\mathbf{L^1H^+(3)}$.

Figure S3. Room-temperature solid-state emission spectrum of $\mathbf{L^2}$ with excitation at 500 nm.

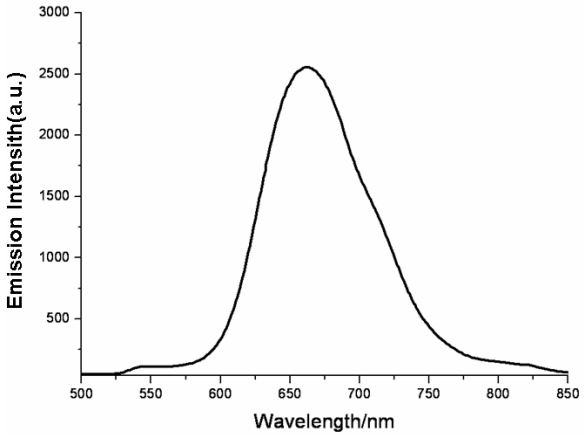


Figure S4. The absorption spectral changes of titration $[Cu(CH_3CN)_4]BF_4$ to $\mathbf{L^1}$ of CH_3OH solution at room

temperature [Cu^+]: 0-0.4 equiv. Inset: [Cu^+]: 0.4-1.0 equiv, final absorption spectrum (dashed dot line) following the addition of PPh_3 in CH_2Cl_2 to the solution of the $[Cu(CH_3CN)_4]BF_4$ titration [PPh_3]: 1.0 equiv.

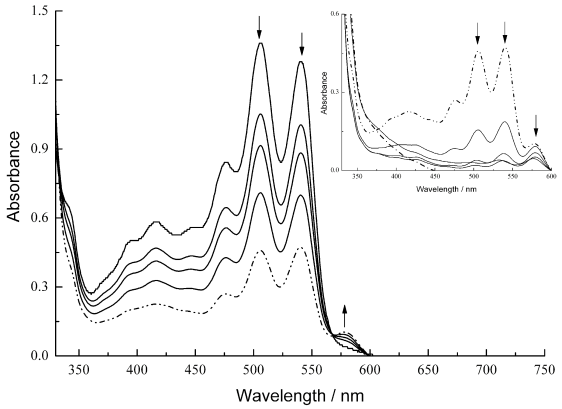


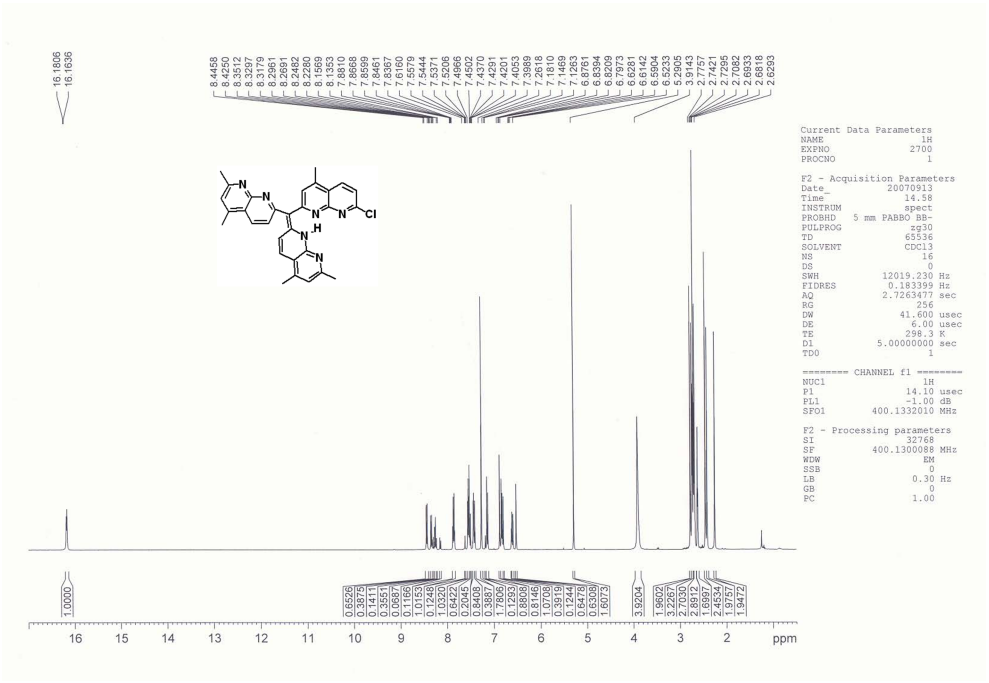
Table S1. Total energies (E_{tot}: a.u) and relative energies (ΔE: kcal·mol^{-1}) for **L^1H^+(1-4)** and **L^1H^+(6)** obtained at the SCRF-B3LYP/6-311++G(d,p) level in CH_2Cl_2 solution.

Species	E_{tot}	ΔE
L^1H^+(3)	-1947.886562	0.0
L^1H^+(4)	-1947.883769	1.8
L^1H^+(2)	-1947.877734	5.5
L^1H^+(6)	-1947.875389	7.0
L^1H^+(1)	-1947.874666	7.5

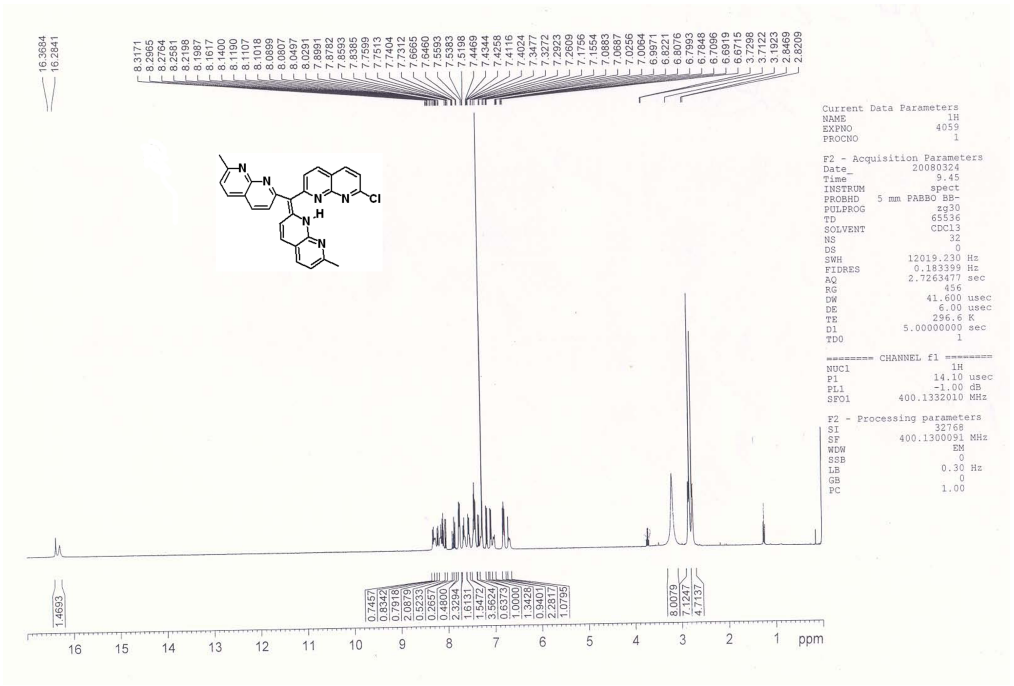
Table S2. Total energies (E_{tot}: a.u) and relative energies (ΔE: kcal·mol^{-1}) for **L^1**, **$L^1_{N(1-4)}$**, **$L^1_{N(6)}$** and **$L^1_{C(10)}$** obtained at the SCRF-B3LYP/6-311++G(d,p) level in CH_2Cl_2 solution.

Species	E_{tot}	ΔE
$L^1_{N(6)}$	-1947.412090	15.9
$L^1_{N(3)}$	-1947.424294	8.3
$L^1_{N(2)}$	-1947.435864	1.0
L^1	-1947.437488	0.0
$L^1_{C(10)}$	-1947.423082	9.0
$L^1_{N(4)}$	-1947.415497	13.8
$L^1_{N(1)}$	-1947.400905	23.0

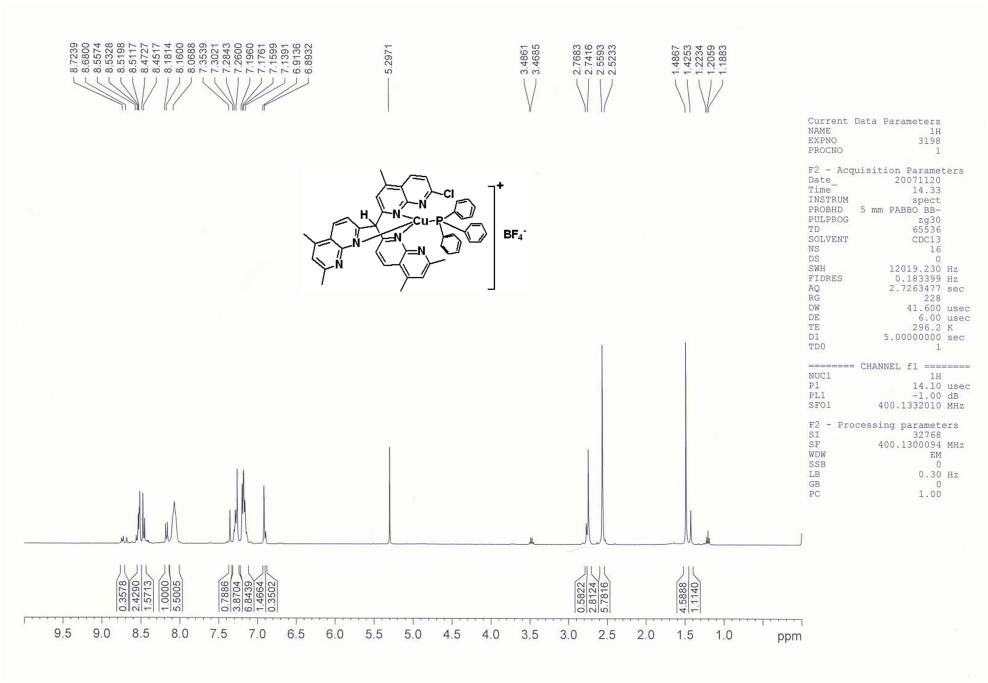
^{1}H-NMR of **L^1**



^{1}H-NMR of **L^2**



^{1}H-NMR of **complex 1**



^{1}H-NMR of **complex 3**