Electronic Supplementary Information

Luminescent mononuclear mixed ligand complexes of copper(I) with 5-phenyl-2,2'-bipyridine and triphenylphosphine

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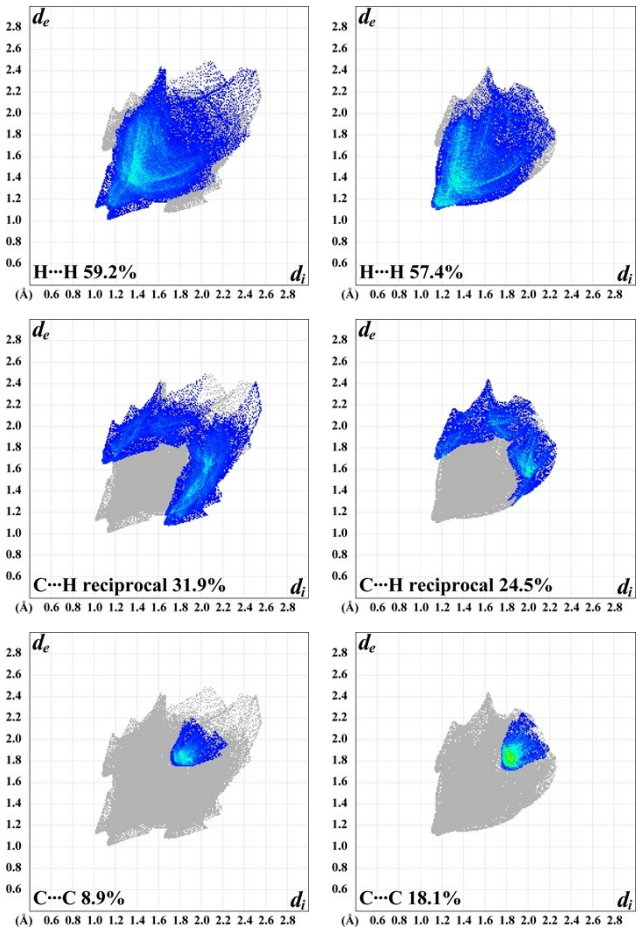


Fig. S1 Decomposed 2D fingerprint plots of observed contacts for the first (left column) and second (right column) molecules of **L**.

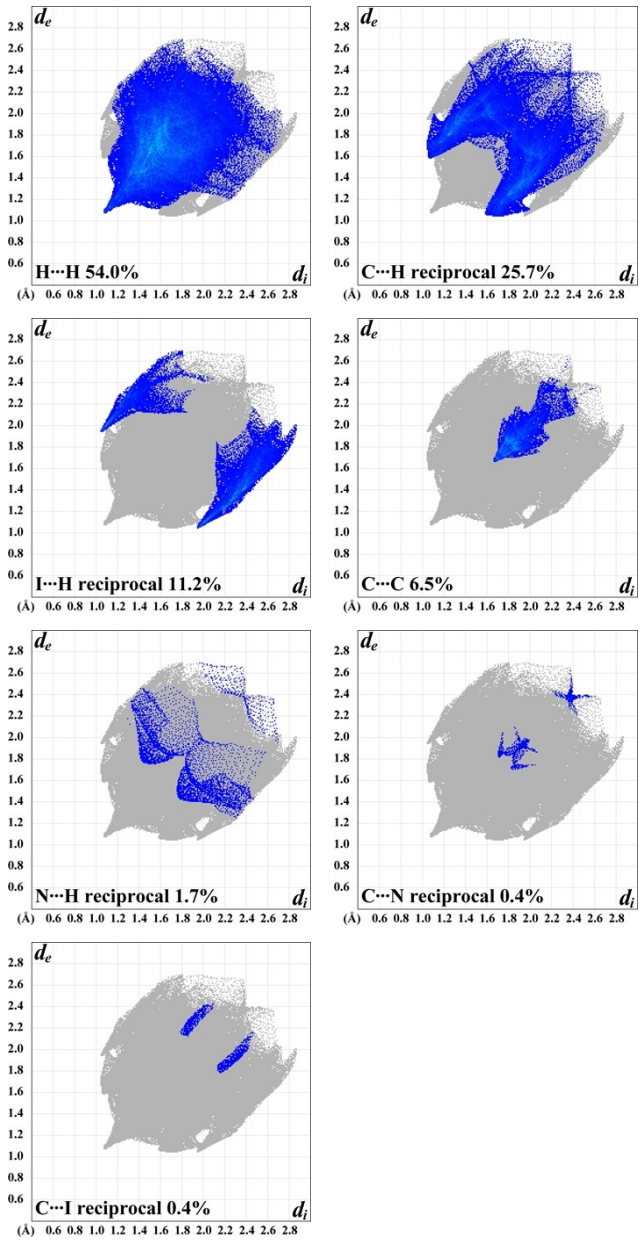


Fig. S2 Decomposed 2D fingerprint plots of observed contacts for **1**.

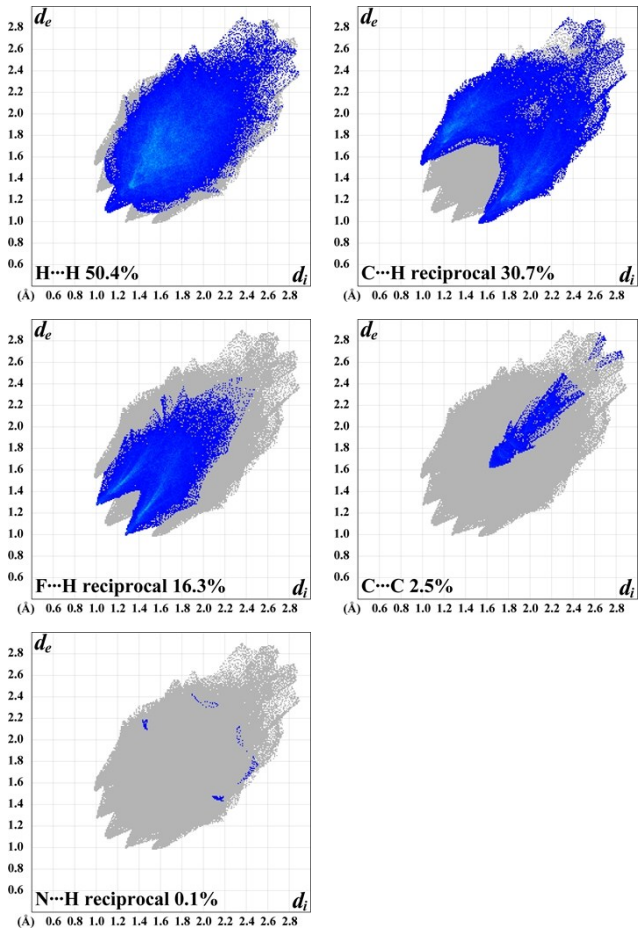
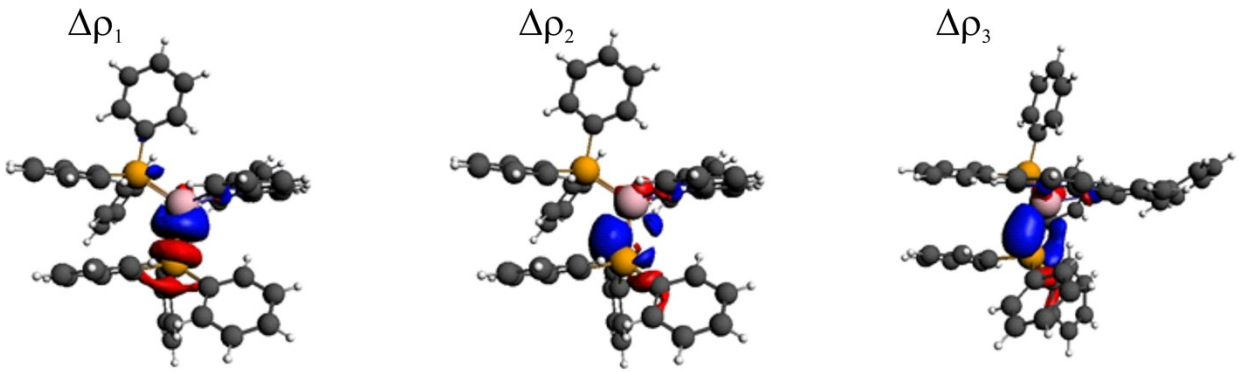


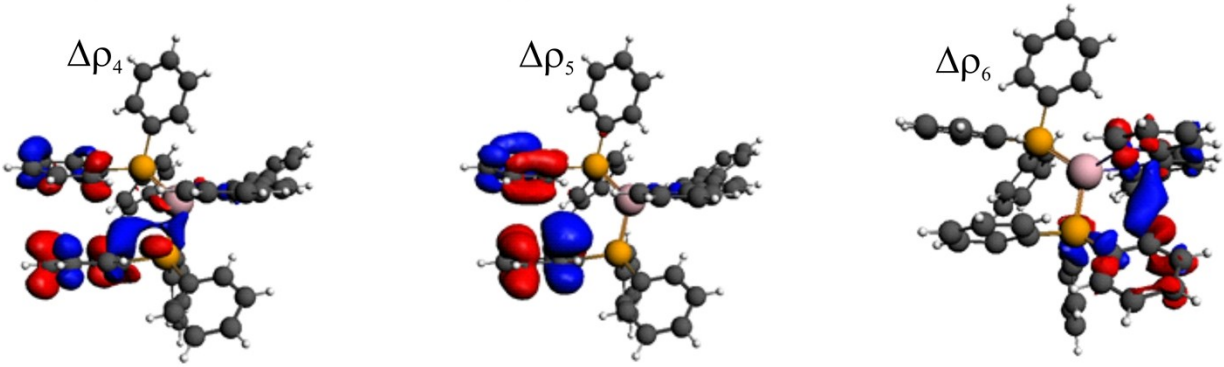
Fig. S3 Decomposed 2D fingerprint plots of observed contacts for **2**.

Dative contributions:



$\Delta E_{orb}(1) = -17.3$ kcal/mol **$\Delta E_{orb}(2) = -5.4$ kcal/mol** **$\Delta E_{orb}(3) = -4.7$ kcal/mol**

Non-covalent Ph···Ph interactions:



$\Delta E_{orb}(4) = -0.54$ kcal/mol **$\Delta E_{orb}(5) = -0.54$ kcal/mol** **$\Delta E_{orb}(6) = -0.4$ kcal/mol**

Fig. S4 The dominant NOCV-based deformation densities, describing the $[CuLPPh_3]–PPh_3$ bond in **2**. The surfaces are plotted at 0.005 a. u. Components are plotted with 0.005 (top row) and 0.0005 (bottom row) a. u., respectively. Red color shows charge depletion, whereas the blue color indicates charge accumulation due to bond formation.

Table S1 The ETS-NOCV energy decomposition results (in kcal/mol), based on DFT/BLYP-D3/TZP, describing bonds in **1** and **2**

	1		**2**	
	$[CuLI]–PPh_3$	$[CuPPh_3I]–L$	$[CuLPPh_3]^+–PPh_3$	$[Cu(PPh_3)_2]^+–L$
ΔE_{elstat}	–114.81	–119.08	–102.25	–128.35
ΔE_{Pauli}	138.20	152.03	125.98	156.62
ΔE_{orb}	–38.96	–50.84	–38.52	–60.56
ΔE_{disp}	–20.30	–18.10	–33.10	–25.16
ΔE_{int}[a]	–35.80	–35.99	–47.89	–57.46

[a] $\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb} + \Delta E_{disp}$