Electronic supplementary information (ESI)

Influence of para substituents in controlling photophysical behavior and different non-covalent weak interactions in zinc complexes of a phenol based "End-off" compartmental ligand

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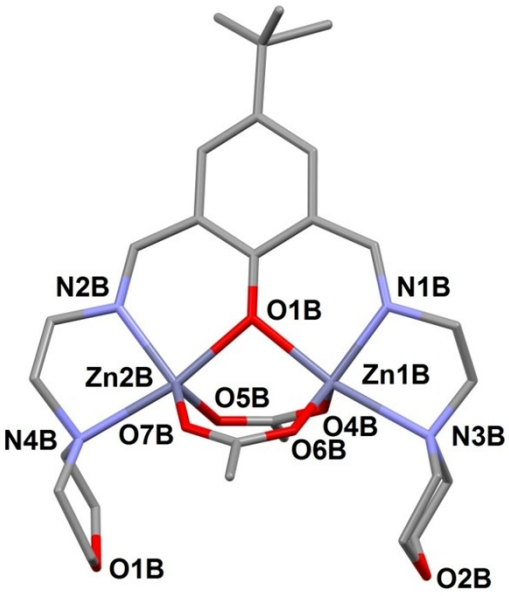

Figure S1. Molecular structure of the$[Zn_2(\mathbf{L\text{-}tbutyl})(CH_3COO)_2]^+$ cation tagged B belonging to compound **2** with the partial atom numbering scheme. Hydrogen atoms have been omitted for clarity.

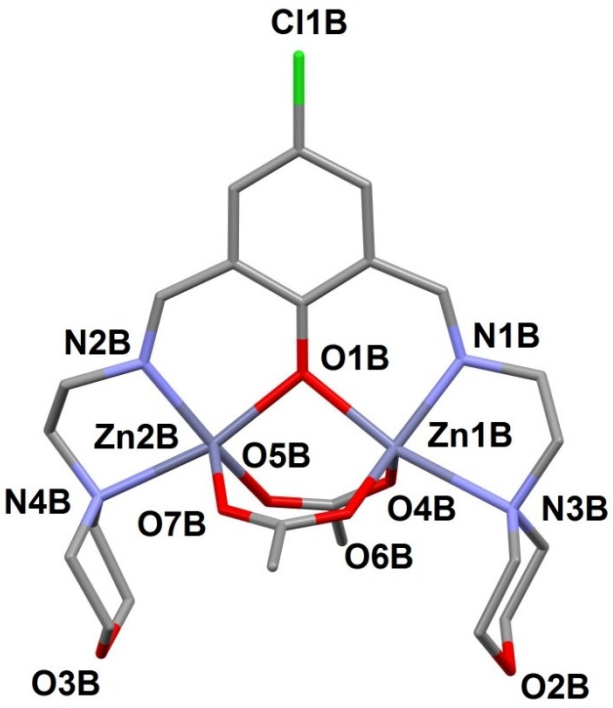

Figure S2. Molecular structure of the $[Zn_2(\mathbf{L\text{-}Cl})(CH_3COO)_2]^+$ cation tagged B belonging to compound **3** with the partial atom numbering scheme. Hydrogen atoms have been omitted for clarity.

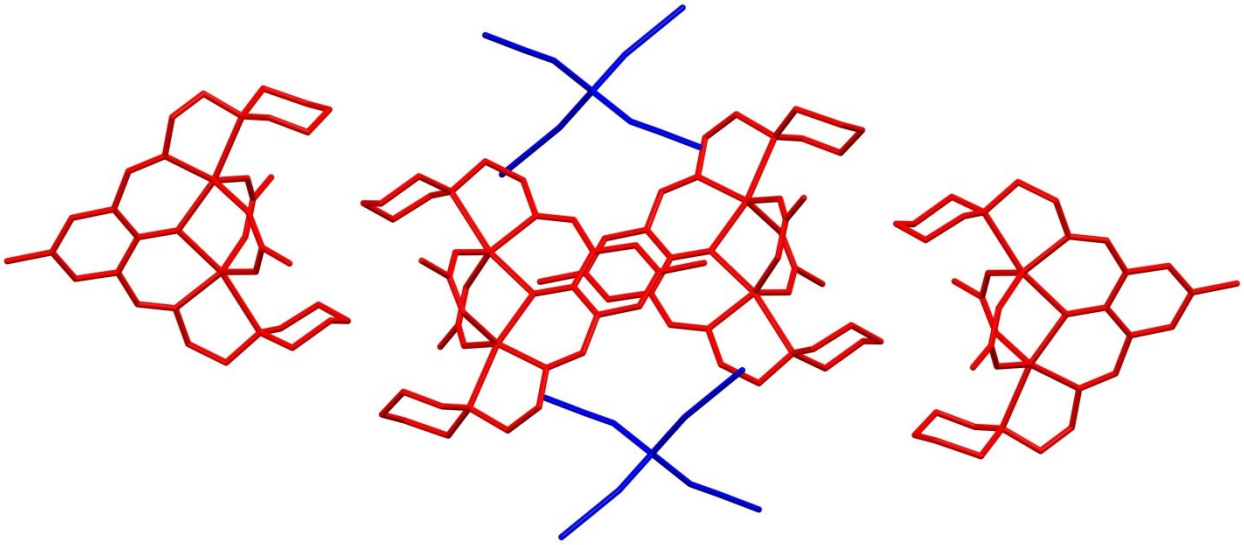

Figure S3. Unit cell content along the cell axis *b* for compound **1**. Complex $[Zn_2(\mathbf{L\text{-}Me})(CH_3COO)_2]^+$, red; $[Zn(SCN)_4]^{2-}$, blue.

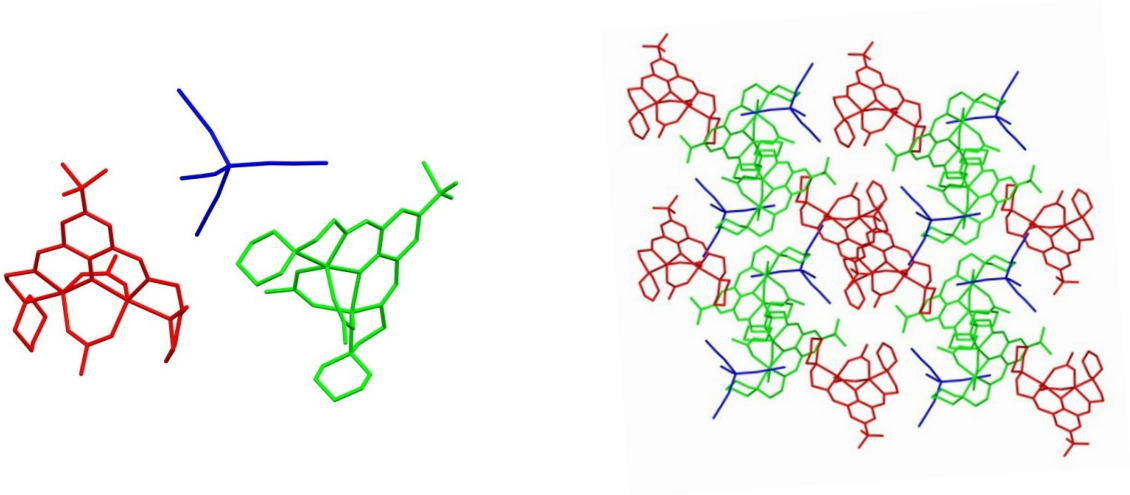

Figure S4. Asymmetric unit (left) and crystal packing along the cell axis *b* (right) for compound **2**. Complex A, green; Complex B, red; $[Zn(SCN)_4]^{2-}$, blue.

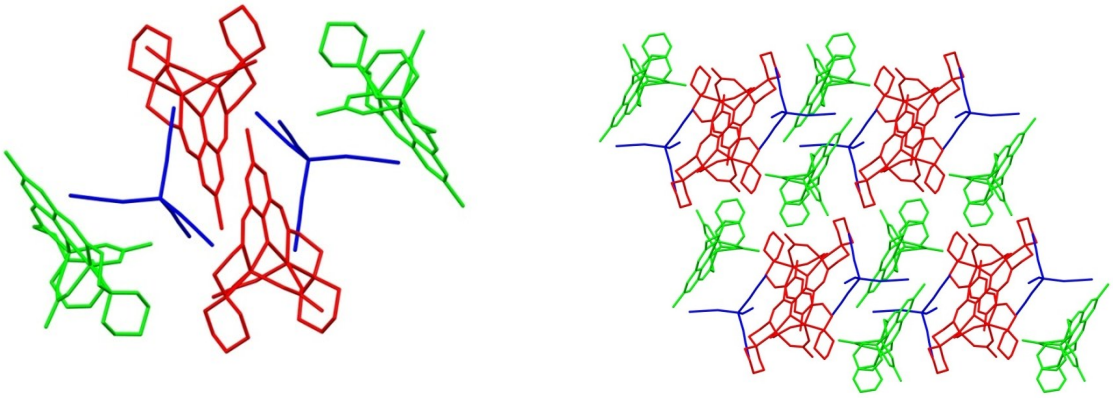

Figure S5. Unit cell content (left) and crystal packing along the cell axis *a* (right) for compound **3**. Complex A, green; Complex B, red; $[Zn(SCN)_4]^{2-}$, blue.

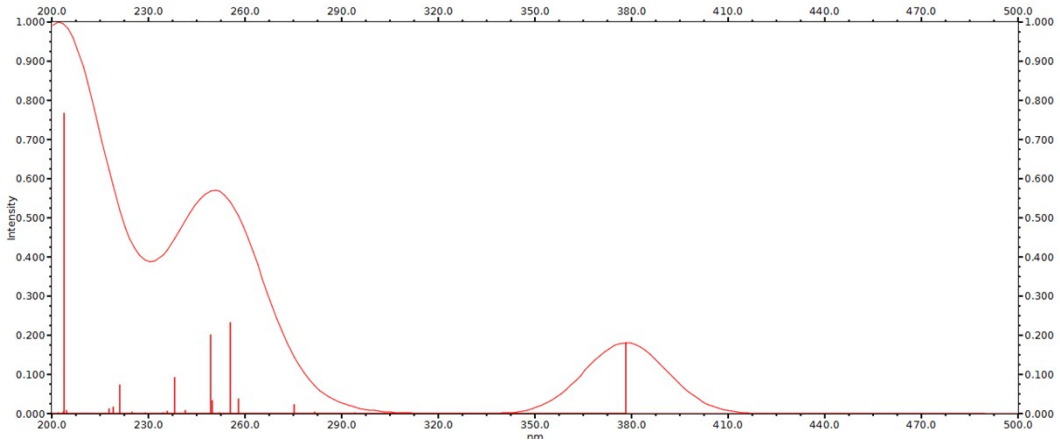

Figure S6. Computed PCM-TD-B3LYP UV-Vis absorption spectrum of Complex **1 (Cl)**. The theoretical spectrum is convoluted with a Gaussian function with a full width at half-maximum (fwhm) of 15 nm; the corresponding transitions are marked with vertical lines.

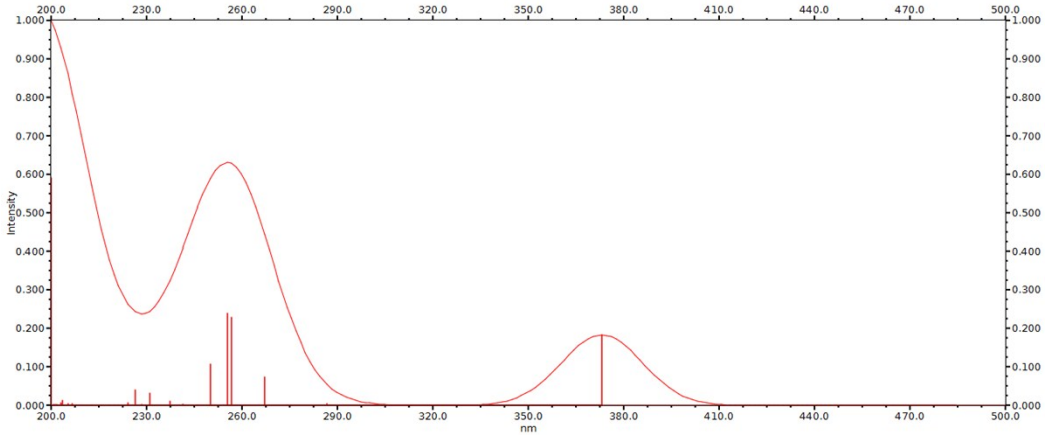

Figure S7. Computed PCM-TD-B3LYP UV-Vis absorption spectrum of Complex **2**. The theoretical spectrum is convoluted with a Gaussian function with a full width at half-maximum (fwhm) of 15 nm; the corresponding transitions are marked with vertical lines.

Table S1. Absorption and steady state fluorescence data of three complexes in methanol : dichloromethane - 1:1 (v/v) mixed solvent at 298K.

Complex	$\lambda_{max}^{(A)}$ **(nm)** **ε ($M^{-1}cm^{-1}$)**		$\lambda_{max}^{(F)}$ **(nm)** **[λ_{ex}=390nm]**
1	260.0 (5746.0)	392.0 (1966.0)	447.0
2	261.0 (16690.0)	389.0 (5450.0)	443.0
3	254.0 (5480.0)	394.0 (1860.0)	455.0

Table S2. Relative quantum yield in fluorescence and phosphorescence spectra

Complex	**Relative Fluorescence quantum yield With respect to Complex 3**	**Relative Phosphorescence quantum yield With respect to Complex 2**
1	0.77	0.81
2	0.72	1.00
3	1.00	0.54