Electronic Supplementary Information

Ligand Influence Versus Electronic Configuration of d-metal Ion in Determining the Fate of NIR Emission from Ln^{III} Ions: A Case Study with Cu^{II}, Ni^{II} and Zn^{II} Complexes.

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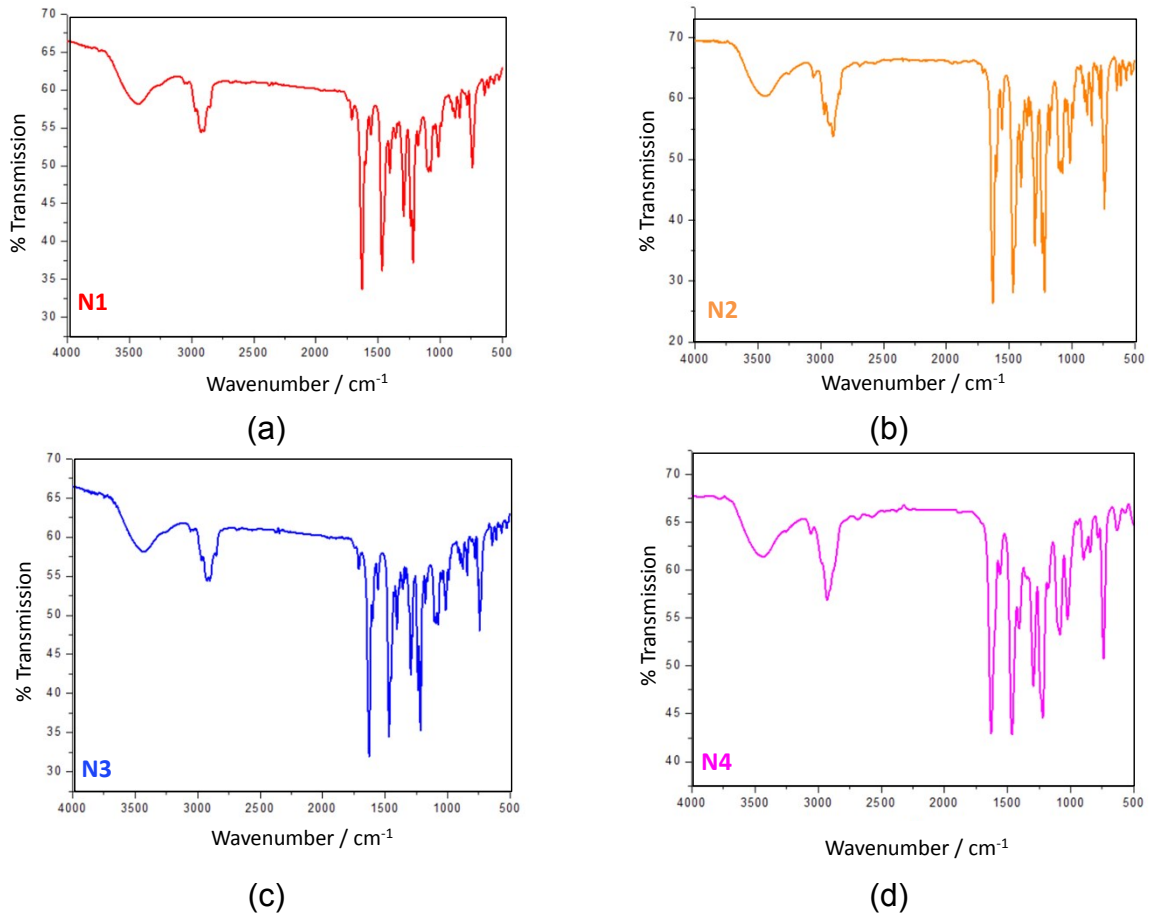

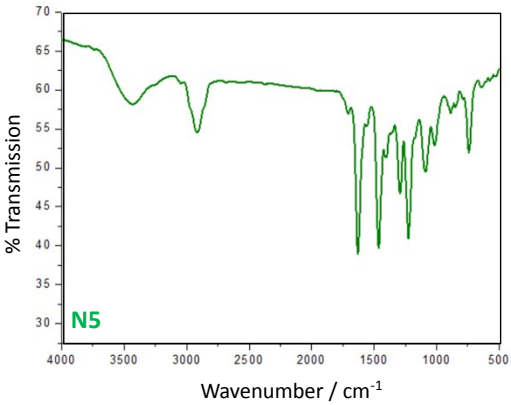
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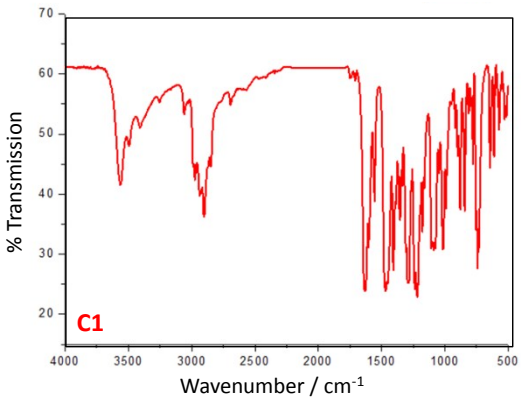
N5
Wavenumber / cm-1

(e)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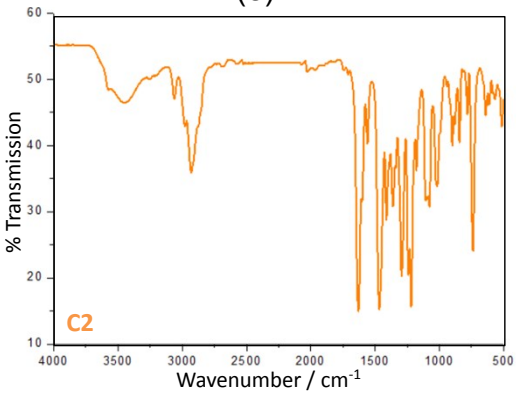
(f)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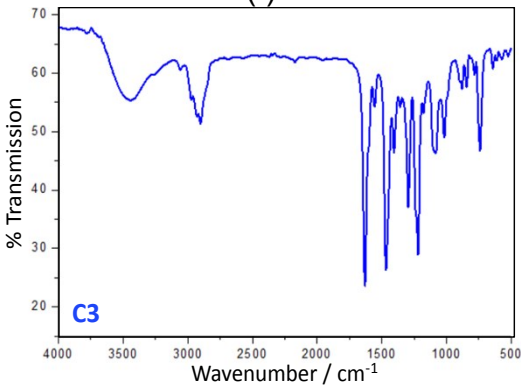
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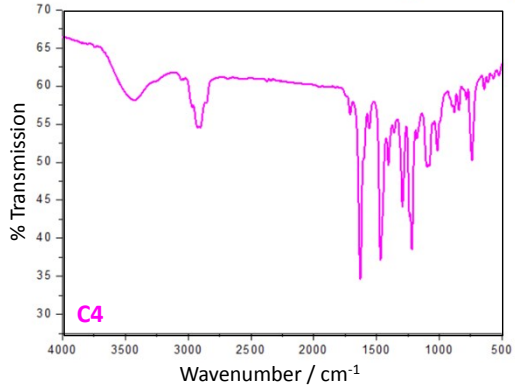
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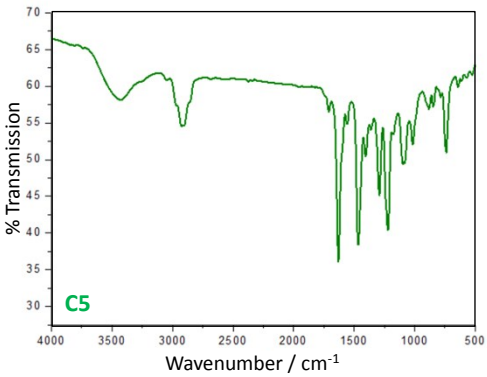
(i)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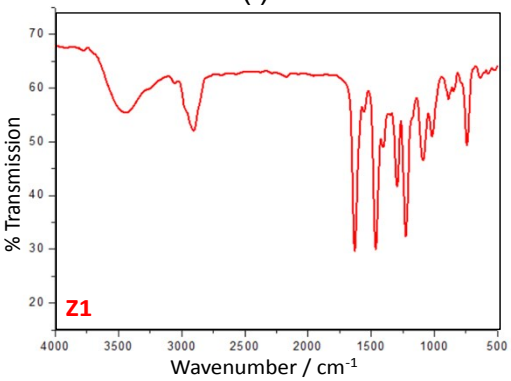
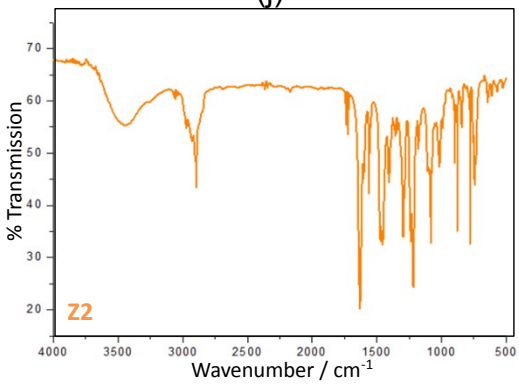

% Transmission
Z1
Wavenumber / cm-1

(k)


% Transmission
Z2
Wavenumber / cm-1

(l)

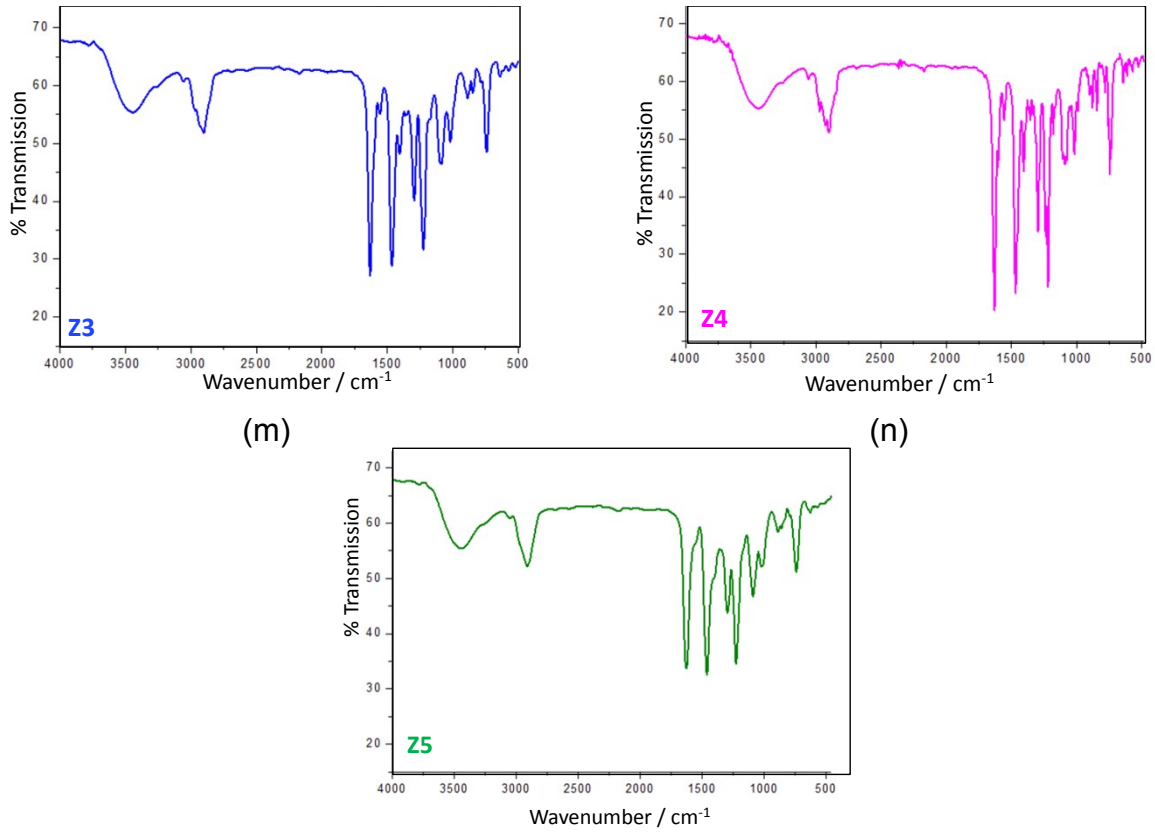


Figure S1. FT-IR spectra (a-e) for [**L-Ni-Ln**], (f-j) for [**L-Cu-Ln**] and (k-o) for [**L-Zn-Ln**] complexes.

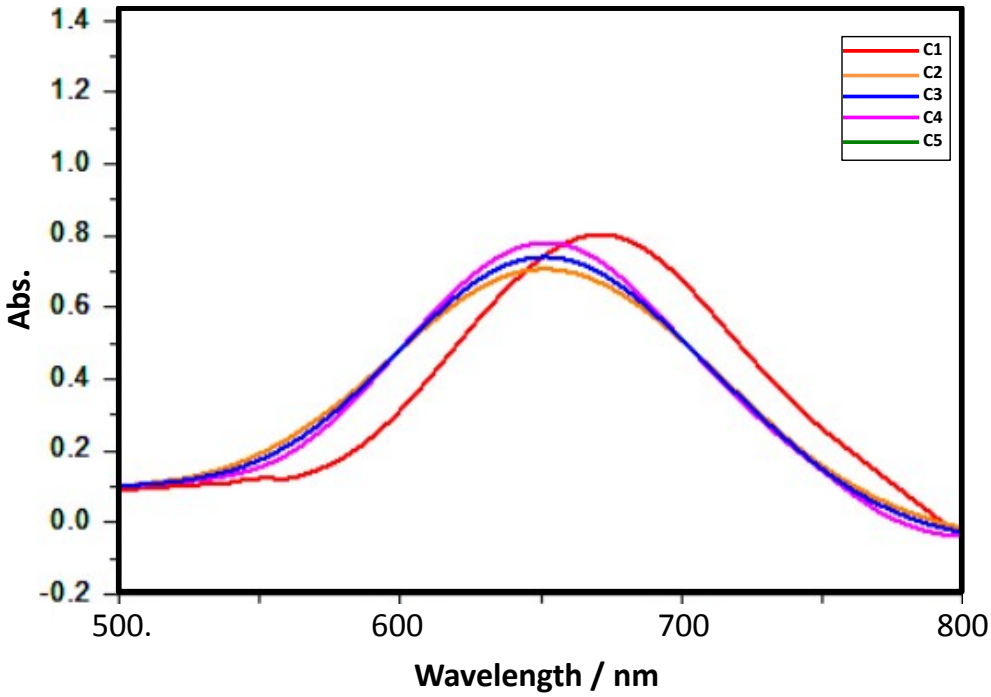
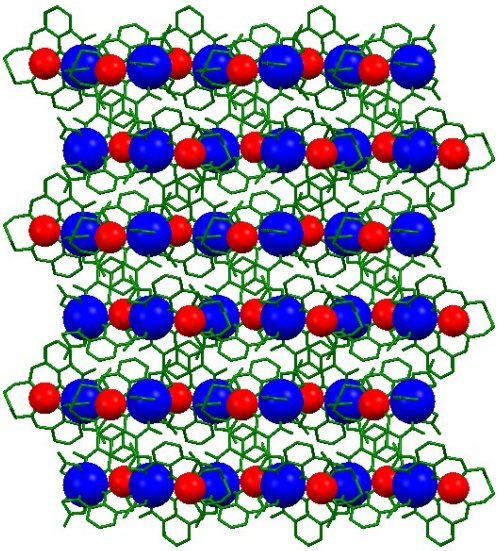
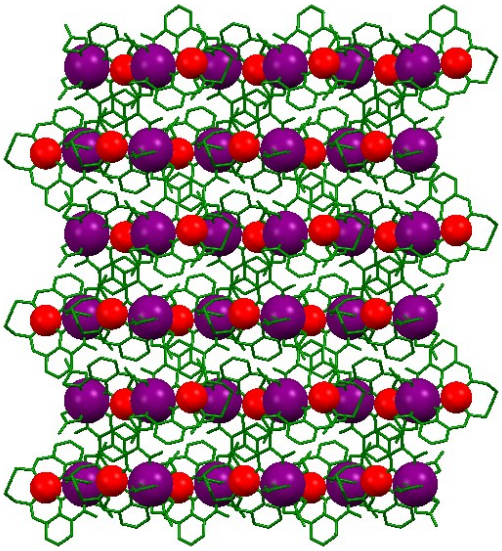


Figure S2. UV-Visible spectra for [**L-Cu-Ln**] complexes at higher concentration (~2 X 10^{-4} M)



(a)



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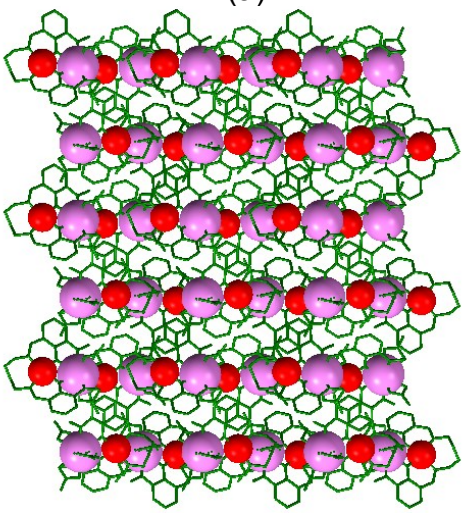
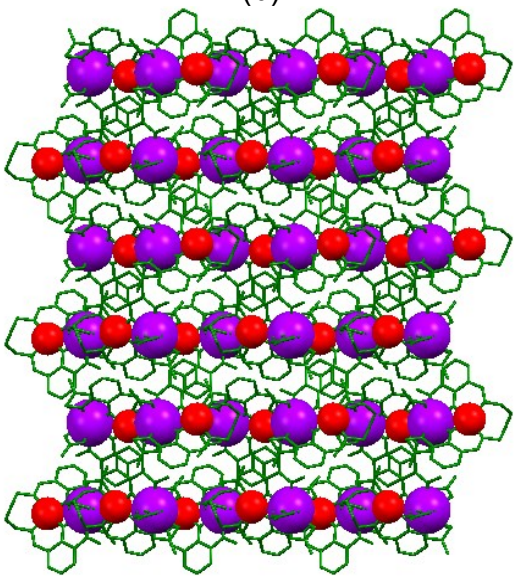
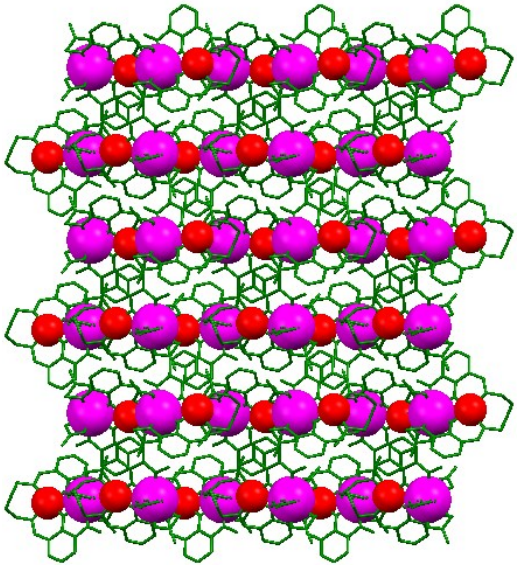


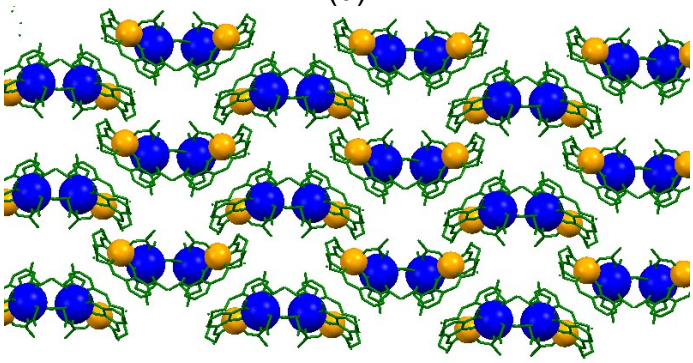
(c)



(d)



(e)



(f)

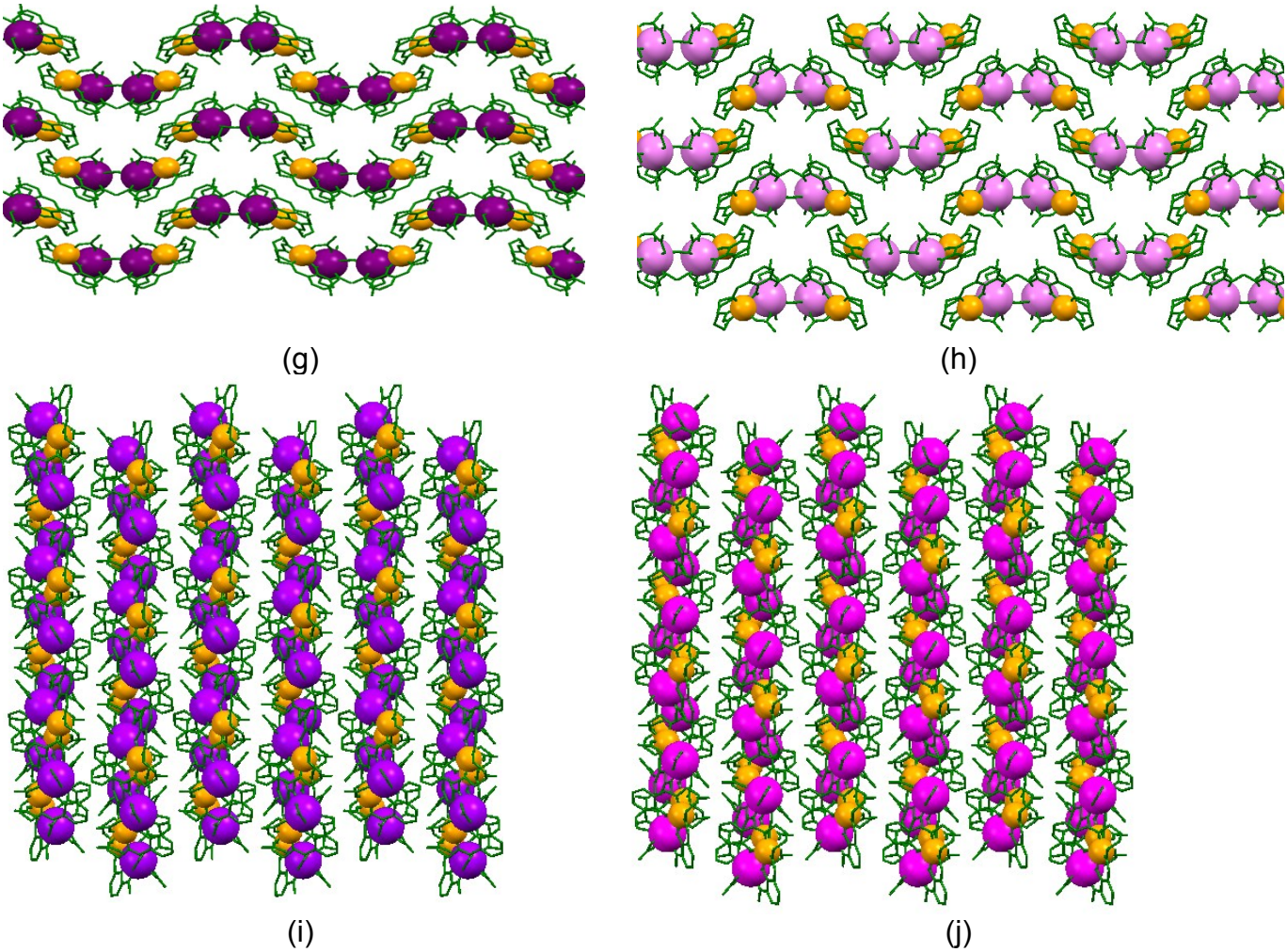
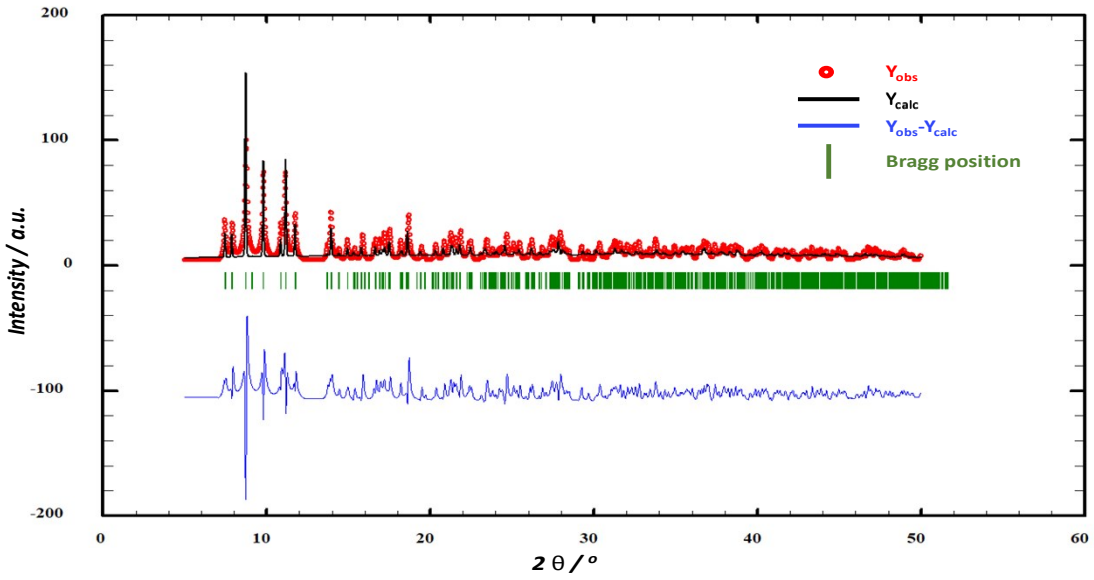
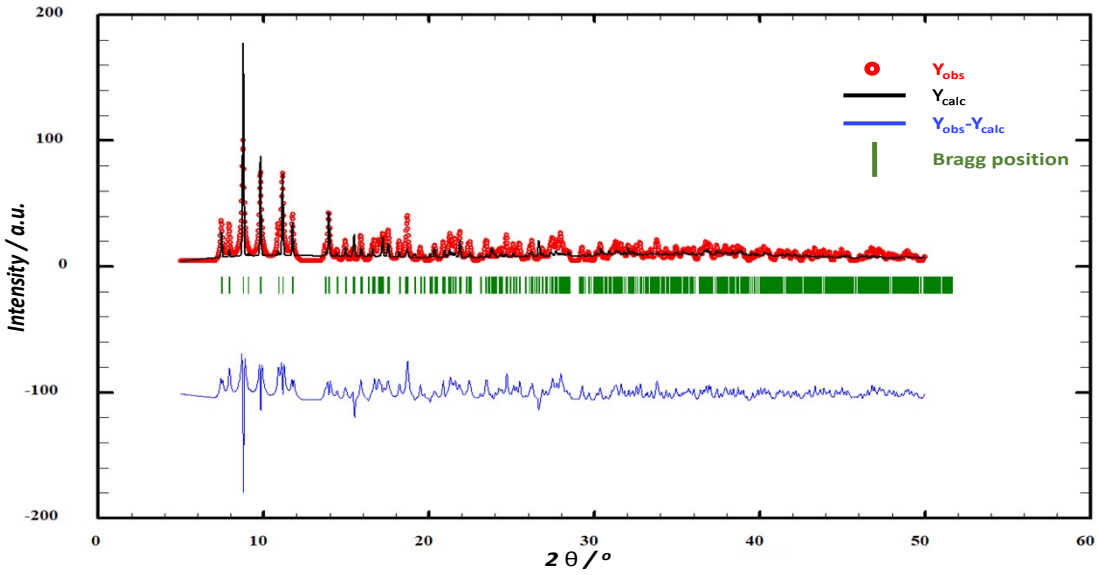


Figure S3. Packing diagram for [**L-Cu-Ln**] complexes (a) [**C1**]; (b) [**C2**]; (c) [**C3**]; (d) [**C4**]; (e) [**C5**] and for [**L-Zn-Ln**] complexes (f) [**Z1**]; (g) [**Z2**]; (h) [**Z3**]; (i) [**Z4**]; (j) [**Z5**] down the b-axis.



(a)



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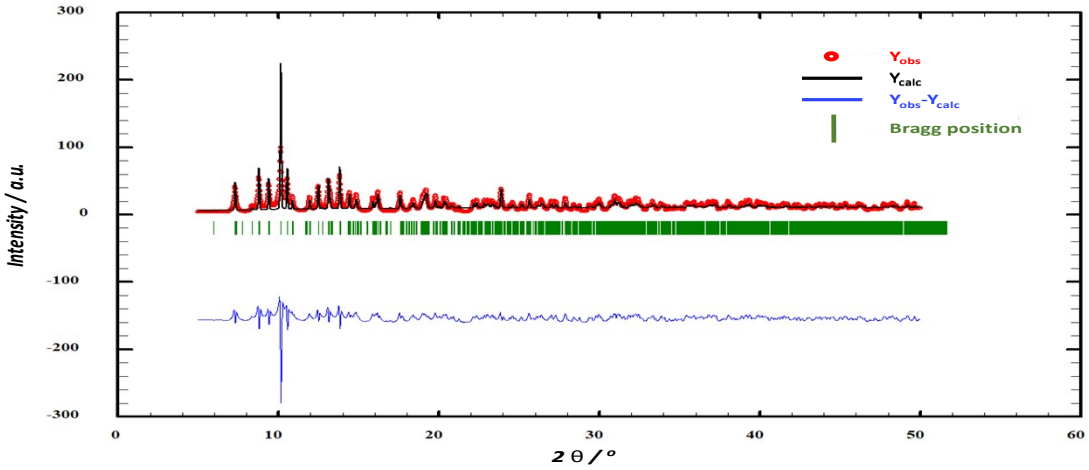

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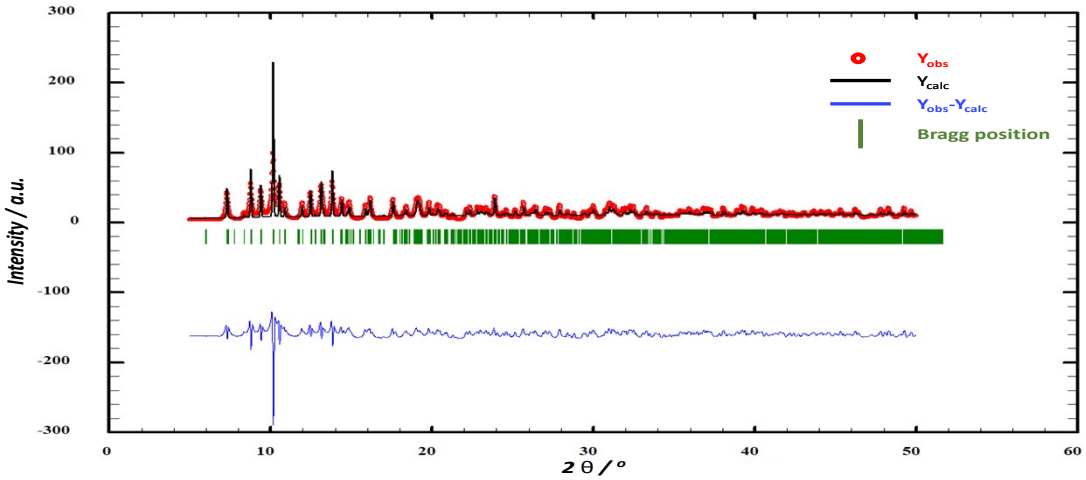
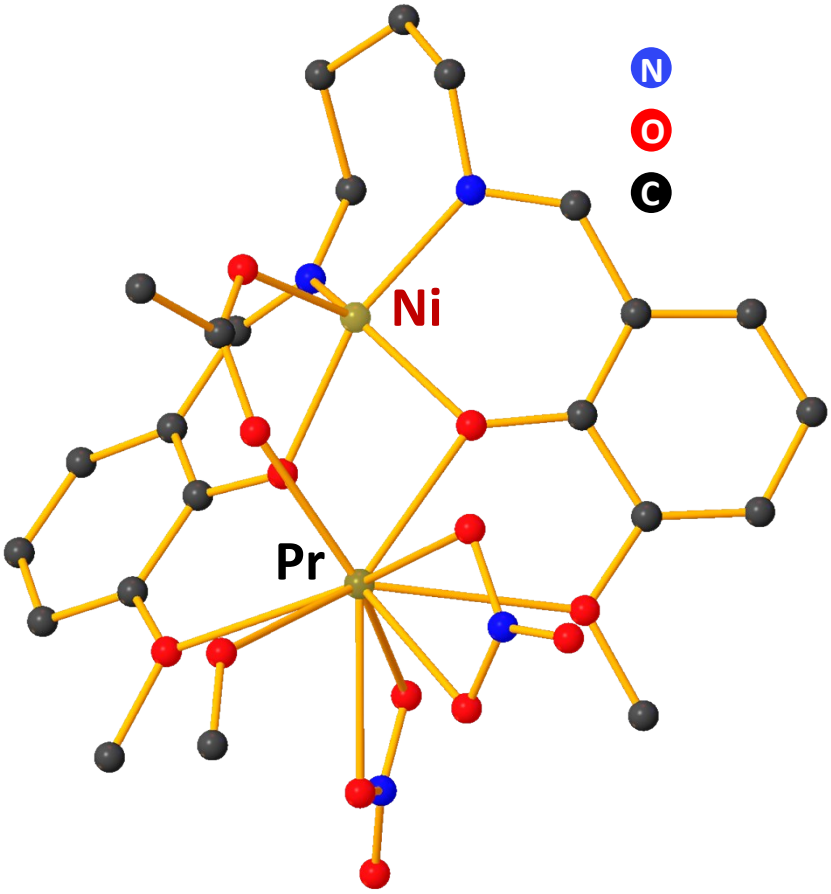


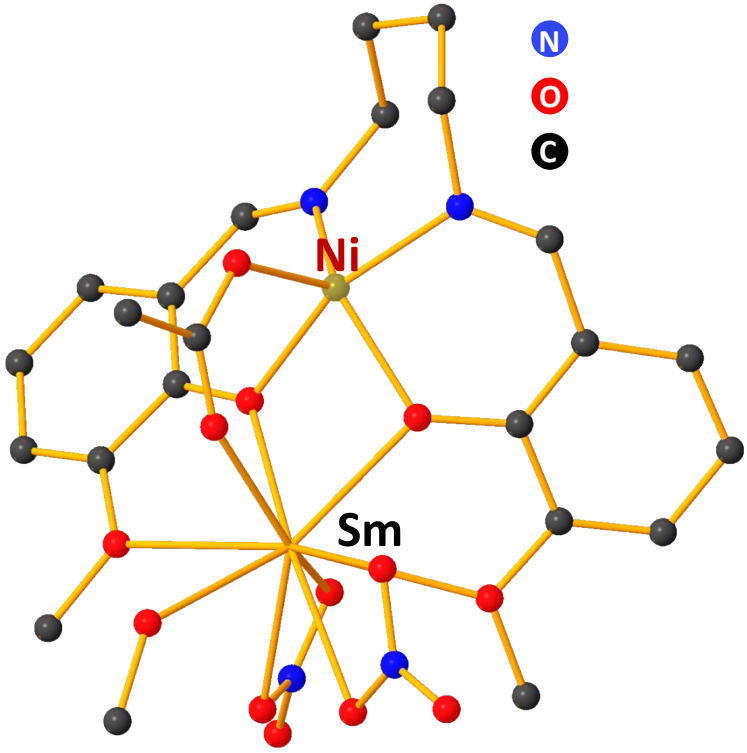
(d)

Figure S4. Rietveld refined PXRD patterns for the [**L-Ni-Ln**] complexes (a to d for [**N2**] to [**N5**] respectively). [N1] is discussed in the main manuscript. The red dots represent experimental points, and the solid black line represents Rietveld refined data. The bottom blue line shows the difference between the experimental and refined data. The marked 2θ positions are the allowed

Bragg peaks.



(a)



(b)

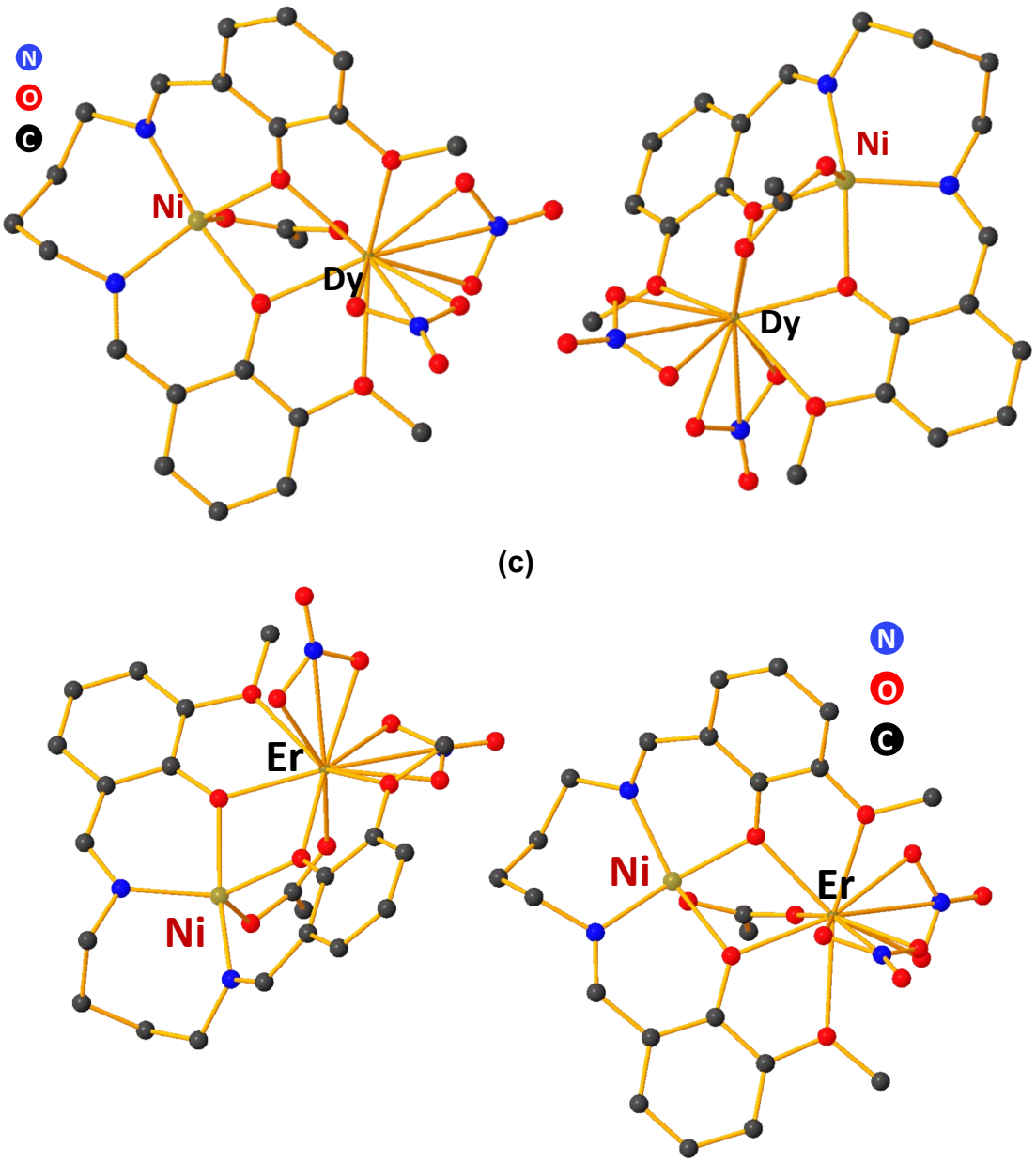


Figure S5. The structures generated from Rietveld refinement using experimental PXRD patterns of the [**L-Ni-Ln**] complexes. (a) [**L-Ni-Pr**], [**N2**]; (b) [**L-Ni-Sm**], [**N3**]; (c) [**L-Ni-Dy**], [**N4**]; (d) [**L-Ni-Er**], [**N5**].

Table S1. Lattice parameters and phase quantification by the Rietveld refinement method for [**L-NI-Ln**] complexes.

Complexes	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	X^2	R_{exp}	R-Factor	D_W-Stat.	R_{wp}	R_p
[**N1**]	12.01	23.69	11.50	90.0	111.88	90.0	1.27	29.7	27.5	0.1025	66.7	78.9
[**N2**]	12.11	23.72	11.48	90.0	112.0	90.0	1.73	29.7	32.8	0.0993	78.7	100
[**N3**]	11.43	23.79	11.89	90.0	111.80	90.0	1.33	29.8	28.4	0.0983	67.6	81.4
[**N4**]	17.83	15.14	20.58	90.0	102.11	90.0	1.28	27.1	24.0	0.1084	63.4	70.3
[**N5**]	17.80	15.13	20.60	90.0	102.02	90.0	1.29	26.8	23.9	0.1062	63.2	70.5