

SUPPLEMENTARY MATERIAL

Allan White and Polypyridines: Extending the Lanthanide(III) Complex Series

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A. Figures S1, S3 and S4 - stick representations of the cations present in the 41 lattices.

B. Figure S2 - Hirshfeld surface diagrams (d_{norm} form from CrystalExplorer) for the cations present in $[\text{Er}(\text{terpy})(\text{OH}_2)_6]\text{Br}_3 \cdot \text{H}_2\text{O}$, **36**, and its known Tm analogue.^[13]

Figure S1 - Cations present in the 1:1 cation:(coordinated ligand) complexes

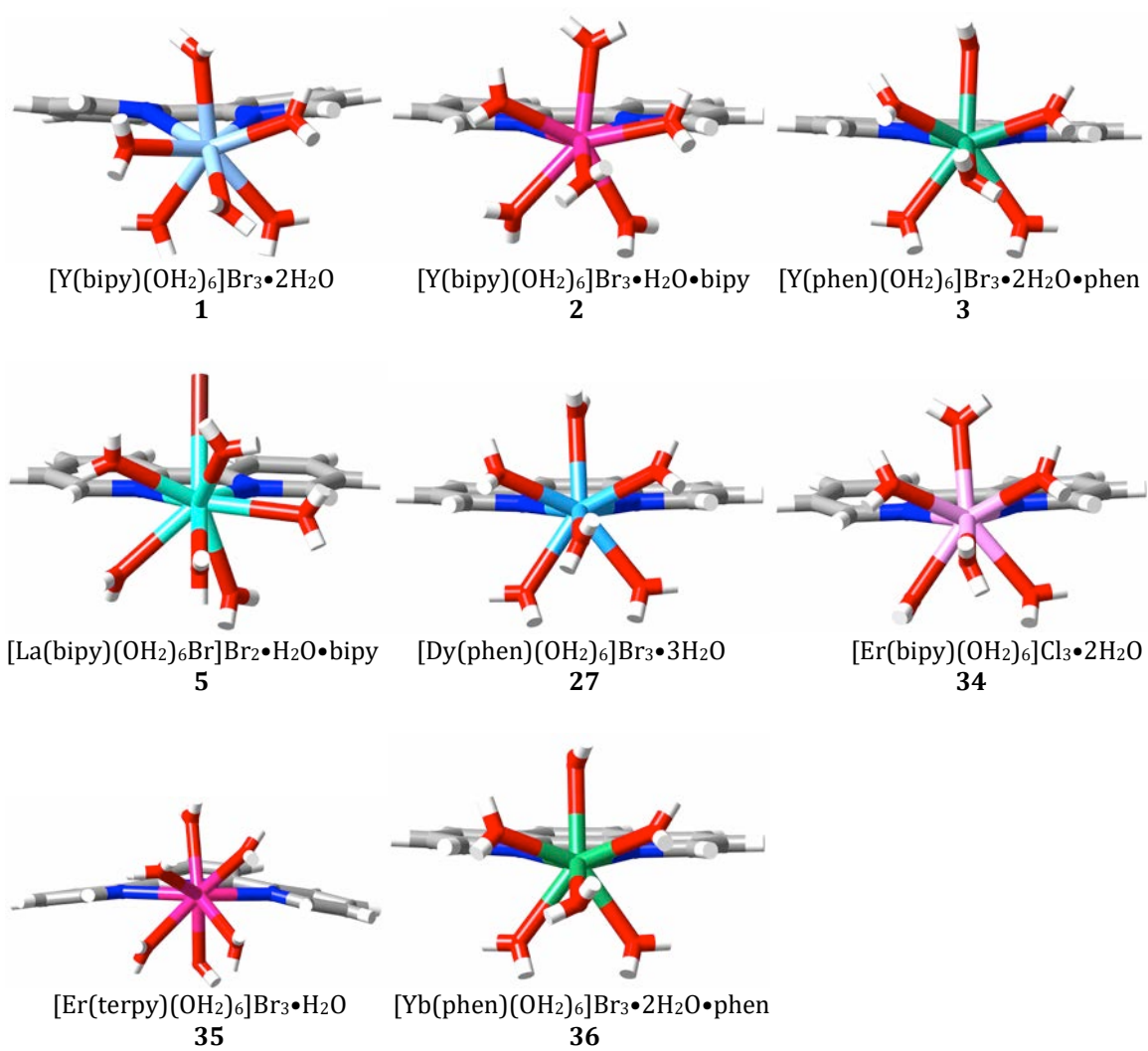


Figure S2 - Hirshfeld surface diagrams (d_{norm} representation) obtained with CrystalExplorer for the cations present in $[\text{Er}(\text{terpy})(\text{OH}_2)_6]\text{Br}_3 \cdot \text{H}_2\text{O}$, **36**, and its known Tm analogue, showing the OH...C interaction (a) with coordinated water of the Er(III) complex and (b) with lattice water in the Tm(III) complex. A red region on the surface designates an area where interaction with an external species exceeds dispersion.

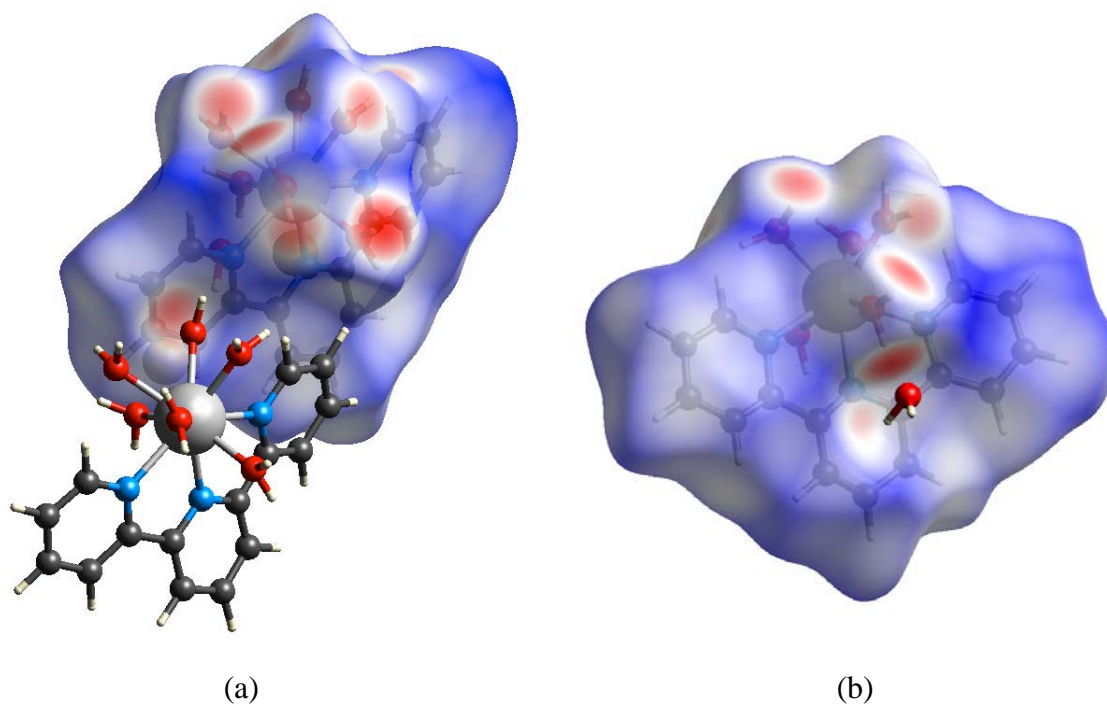
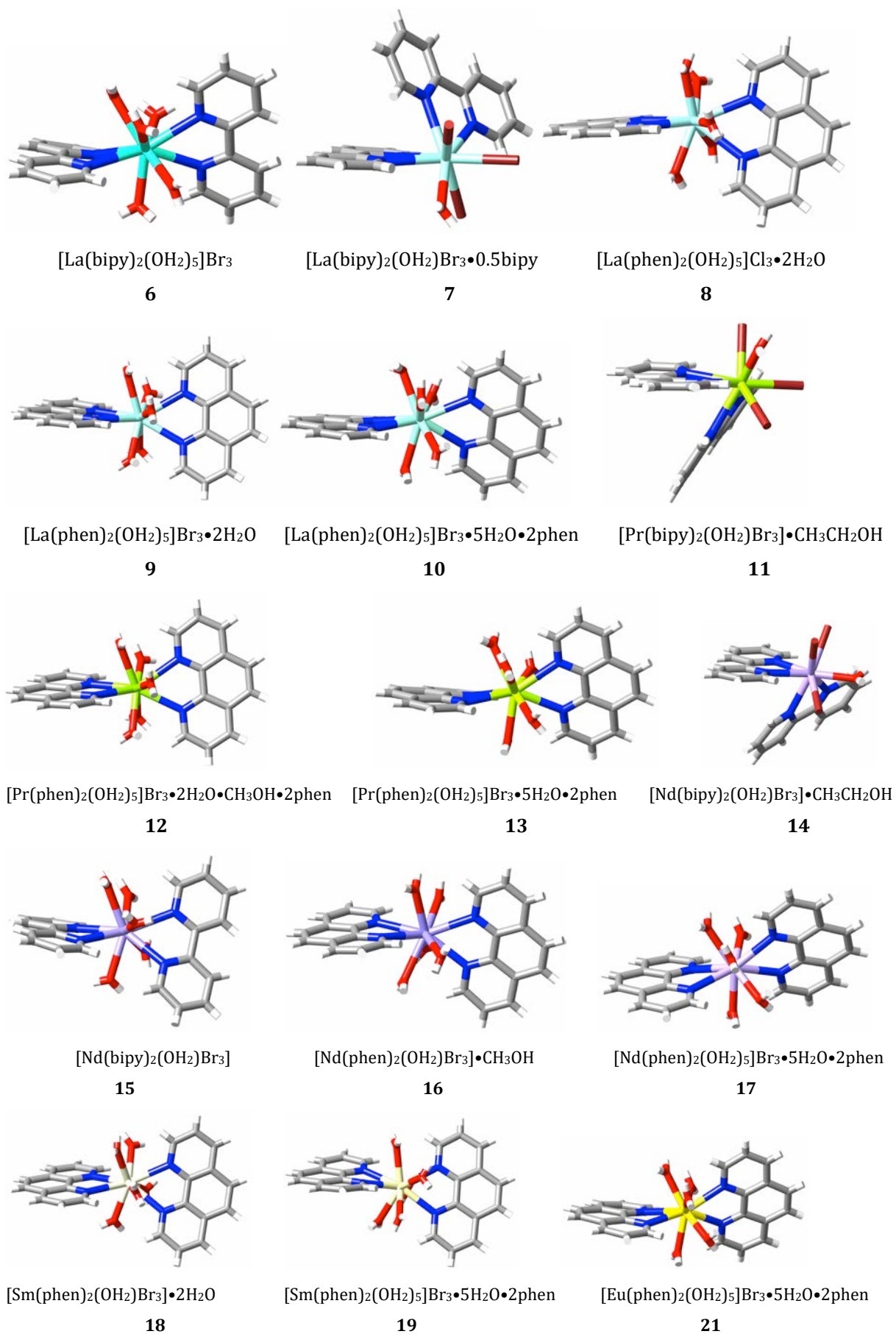
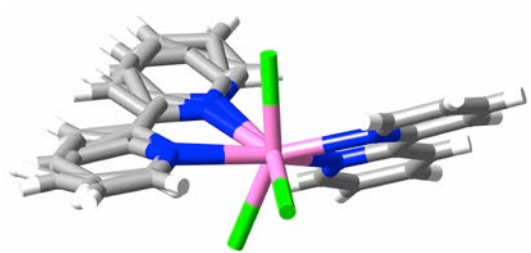


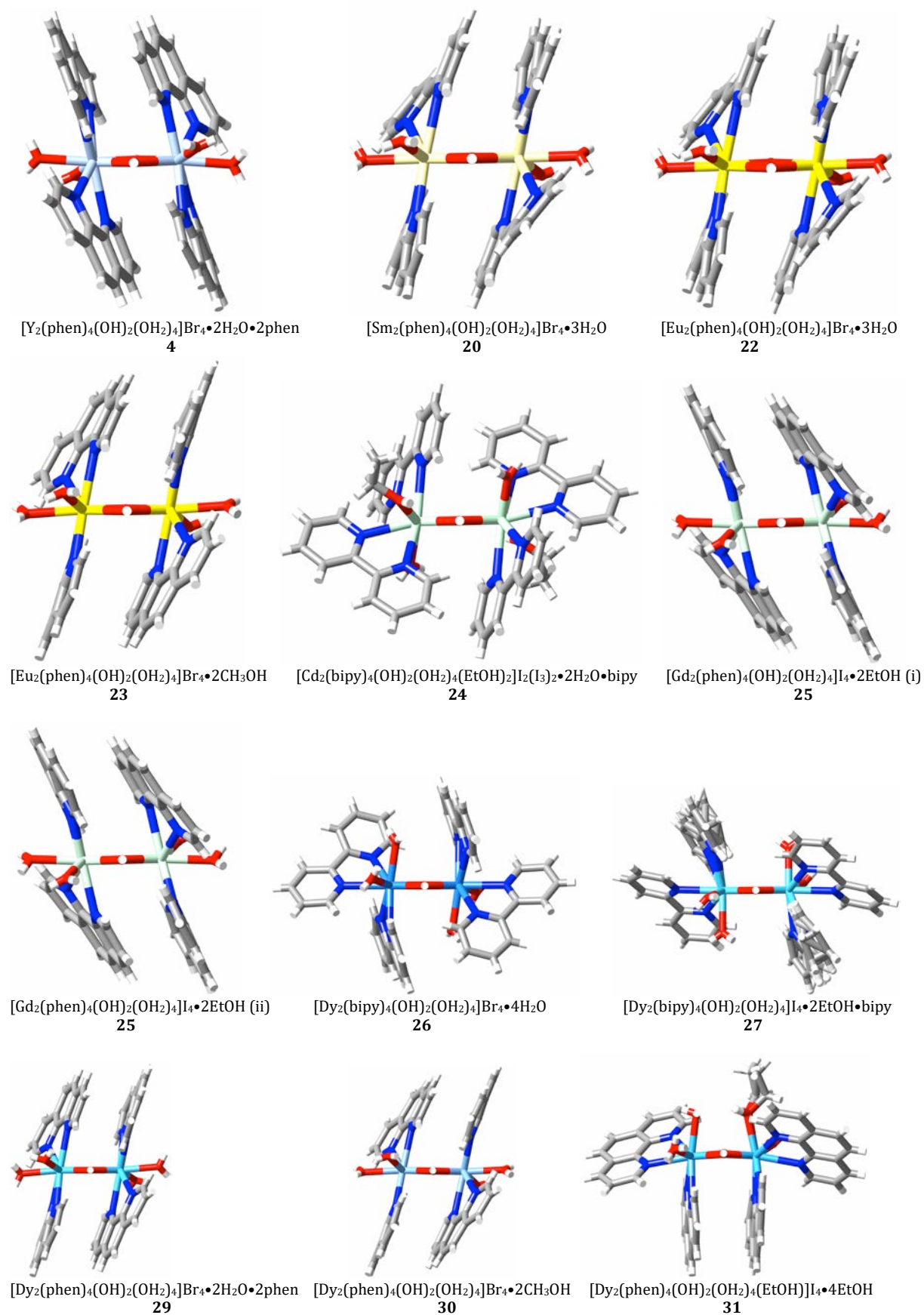
Figure S3 - Cations present in the 1:2 cation:(coordinated ligand) complexes

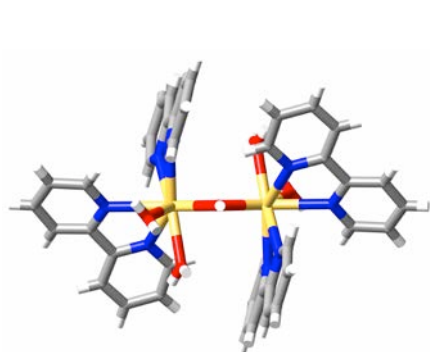




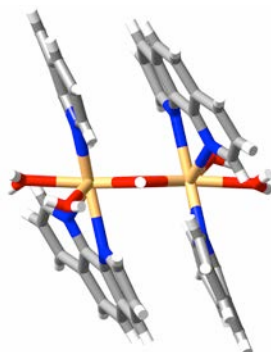
[Er(phen)₂Cl₃] (neutral complex; one phen ligand disordered)

Figure S4 - Cations present in the binuclear 2:4 cation:(coordinated ligand) complexes. Views down the O...O vector of the Ln₂(OH)₂ core.

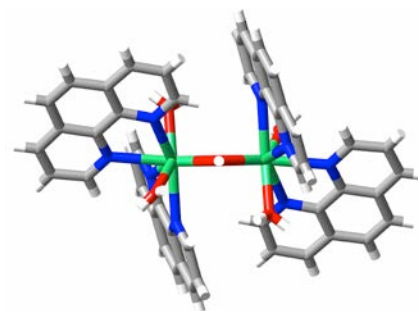




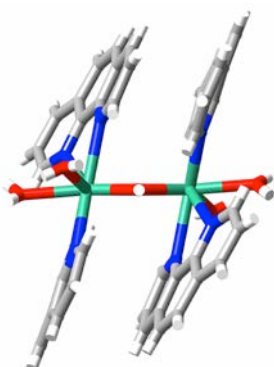
$[\text{Ho}_2(\text{bipy})_4(\text{OH})_2(\text{OH}_2)_4]\text{Br}_4 \cdot 4\text{H}_2\text{O}$
32



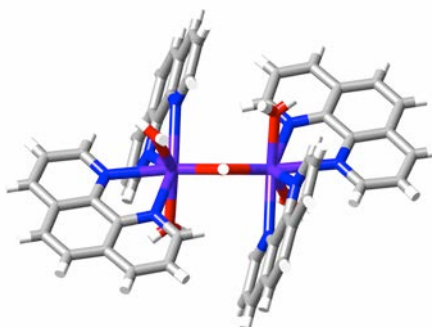
$[\text{Ho}_2(\text{phen})_4(\text{OH})_2(\text{OH}_2)_4]\text{Br}_4 \cdot 2\text{CH}_3\text{OH}$
33



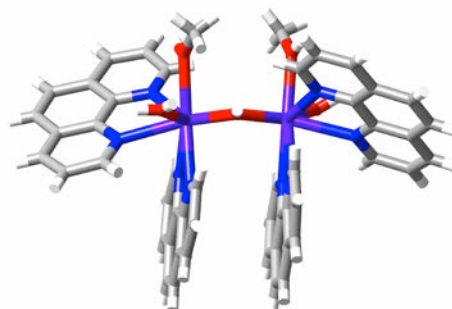
$[\text{Yb}_2(\text{phen})_4(\text{OH})_2(\text{OH}_2)_4]\text{Br}_4 \cdot 12\text{H}_2\text{O} \cdot 2\text{phen}$
38



$[\text{Yb}_2(\text{phen})_4(\text{OH})_2(\text{OH}_2)_4]\text{Br}_4 \cdot 2\text{CH}_3\text{OH}$
39



$[\text{Lu}_2(\text{phen})_4(\text{OH})_2(\text{OH}_2)_4]\text{Br}_4 \cdot 12\text{H}_2\text{O} \cdot 2\text{phen}$
40



$[\text{Lu}_2(\text{phen})_4(\text{OH})_2(\text{OH}_2)_3(\text{MeOH})]\text{Br}_4 \cdot 3.5\text{CH}_3\text{OH}$
41