## **Supporting Information**

## for

## Effect of ionic radius on the assemblies of first row transition metal–5-*tert*-butylisophthalate– (2,2'-bipyridine/phenanthraline) coordination compounds

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Fig. S1 XPRD of  $[Mn_3(tbip)_3(bpy)_2]_n$  and products synthesized at 200 or  $150^{\circ}C$ 



Fig. S2XPRD of  $\{[Mn(tbip)(phen)] \cdot 2H_2O\}_n$  (Simulation 1),  $[Mn(Htbip)_2(phen)_2]$ <br/>(Simulation 2) and products synthesized at 200 or  $150^{\circ}C$ 



Fig. S3 XPRD of [Fe(phen)<sub>3</sub>]·2Htbip·3.5H<sub>2</sub>O



Fig. S4 XPRD of  $\{[Co_3(bpy)_2(tbip)_3Co(bpy)(tbip)]\cdot 5H_2O\}_n$  (Simulation 1),  $[Co(bpy)(tbip)(H_2O)]_4$  (Simulation 2) and products synthesized at 200 or  $150^{\circ}C$ 



Fig. S5 XPRD of  $\{[Co_3(tbip)_3(phen)_2Co(tbip)(phen)]\cdot 1.5H_2O\}_n$  (Simulation 1),  $[Co(tbip)(phen)(H_2O)]_n$  (Simulation 2), TUHFOS and products synthesized at 250 or  $150^{\circ}C$ 



Fig. S6 XPRD of  $[Ni(bpy)(tbip)(H_2O)]_4$  and products synthesized at 200 or  $150^{\circ}C$ 



Fig. S7 XPRD of  $[Ni(tbip)(phen)(H_2O)]_n$  and products synthesized at 200 or  $150^{\circ}C$ 







Fig. S9 XPRD of  $[Cu(tbip)(phen)(H_2O)]$  (Simulation 1),  $[Cu(Htbip)_2(phen)]_n$ (Simulation 2),  $[Cu(tbip)(H_2tbip)(phen)]_n$  (Simulation 3) and products



Fig. S10 XPRD of [Zn(bpy)(tbip)(H<sub>2</sub>O)]<sub>4</sub> and products synthesized at 200 or 150°C



Fig. S11XPRD of { $[Zn(phen)(tbip)(H_2O)] \cdot 0.5H_2O$ }<sub>n</sub> (Simulation 1),{ $[Zn(phen)(tbip)(H_2O)] \cdot H_2O$ }<sub>n</sub> (Simulation 2),  $[Zn(tbip)(H_2tbip)(phen)]_n$ (Simulation 3) and products synthesized at 200 or 150°C