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# Supporting Information

## Two- and Three-Dimensional Lanthanide-Based Coordination Polymers Assembled by the Synergistic Effect of Various Lanthanide Radii and Flexibility of a New Binicotinate-Containing Ligand: in Situ Synthesis, Structures, and Properties

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**The IR data**

Polymer **[La(hbptcH)($H_2O$)]$_n$** (**1**): IR (KBr, $cm^{-1}$): 3489-3074(b), 1565(s), 1533(s), 1483(m), 1408(m), 1365(s), 1317(s), 1276(S), 1253(S), 1172(m), 1096(m), 994(m), 941(w), 870(s), 830(s), 807(s), 725(s), 686(S).

Polymer **[Ce(hbptcH)($H_2O$)]$_n$** (**2**): IR (KBr, $cm^{-1}$): 3488-3072(b), 1566(s), 1533(s), 1483(m), 1409(m), 1366(s), 1317(s), 1275(S), 1254(S), 1171(m), 1097(m), 995(m), 940(w), 870(s), 831(s), 807(s), 726(s), 686(S).

Polymer **[Pr(hbptcH)($H_2O$)]$_n$** (**3**): IR (KBr, $cm^{-1}$): 3486-3073(b), 1566(s), 1533(s), 1483(m), 1408(m), 1365(s), 1318(s), 1276(S), 1252(S), 1173(m), 1097(m), 995(m), 941(w), 870(s), 830(s), 807(s), 726(s), 686(S).

Polymer **[Eu(hbptcH)($H_2O$)$_2$]$_n$** (**4**): IR (KBr, $cm^{-1}$): 3485-3073(b), 1576(s), 1549(m), 1393(s), 1367(s), 1334(m), 1228(s), 1211(S), 1183(m), 1162(m), 1146(m), 1113(m), 1092(m), 984(w), 918(s), 871(m), 852(s), 804(s), 728(s), 676(S).

Polymer **[Gd(hbptcH)($H_2O$)$_2$]$_n$** (**5**): IR (KBr, $cm^{-1}$): 3483-3063(b), 1577(s), 1550(m), 1391(s), 1369(s), 1335(m), 1230(s), 1213(S), 1185(m), 1147(m), 1112(m), 1093(m), 985(w), 910(s), 872(m), 852(s), 804(s), 727(s), 679(S).

Polymer **[Tb(hbptcH)($H_2O$)$_2$]$_n$** (**6**): IR (KBr, $cm^{-1}$): 3482-3065(b), 1575(s), 1552(m), 1390(s), 1367(s), 1336(m), 1232(s), 1215(S), 1183(m), 1146(m), 1114(m), 1092(m), 986(w), 911(s), 874(m), 853(s), 802(s), 729(s), 678(S).

Polymer **[Dy(hbptcH)($H_2O$)$_2$]$_n$** (**7**): IR (KBr, $cm^{-1}$): 3489-3055(b), 1575(s), 1549(m), 1389(s), 1368(s), 1335(m), 1271(m), 1229(s), 1212(S), 1184(m), 1147(m), 1113(m), 1092(m), 985(w), 912(s), 871(m), 851(s), 804(s), 727(s), 676(S).

Polymer **[Ho(hbptcH)($H_2O$)$_2$]$_n$** (**8**): IR (KBr, $cm^{-1}$): 3489-3053(b), 1576(s), 1552(m), 1387(s), 1369(s), 1337(m), 1272(m), 1228(s), 1211(S), 1183(m), 1146(m), 1112(m), 1092(m), 984(w), 912(s), 873(m), 852(s), 804(s), 728(s), 677(S).

Polymer **[Er(hbptcH)($H_2O$)$_2$]$_n$** (**9**): IR (KBr, $cm^{-1}$): 3490-3051(b), 1577(s), 1552(m), 1390(s), 1369(s), 1335(m), 1274(m), 1230(s), 1213(S), 1185(m), 1148(m), 1112(m), 1093(m), 985(w), 910(s), 872(m), 852(s), 804(s), 727(s), 679(S).

Polymer **[Lu(hbptcH)($H_2O$)$_2$]$_n$** (**10**): IR (KBr, $cm^{-1}$): 3491-3047(b), 1578(s), 1555(m), 1394(s), 1370(s), 1338(m), 1232(s), 1214(S), 1184(m), 1148(m), 1111(m), 1095(m), 990(w),

914(m), 872(m), 852(s), 804(s), 729(s), 682(S).

**Table S1**. **Geometrical parameters of hydrogen bonds in 1–3**[a]

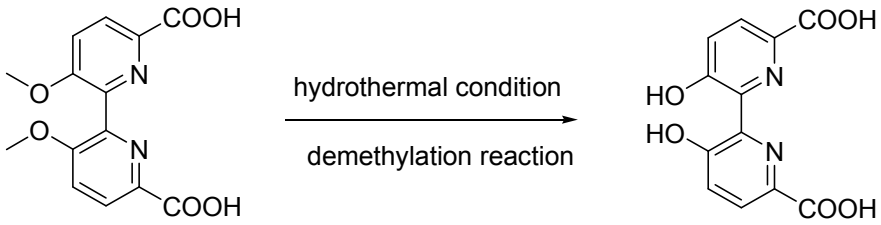
| Bond | | Distance (Å) | | |
|---|---|---|---|---|
| | | 1·La | 2·Ce | 3·Pr |
| O(6)–H···O(3) | O···O distance | 2.460(3) | 2.459(4) | 2.459(4) |
| hydrogen bond | O–H···O angle | 167.3 | 164.7 | 167.5 |
| O(7)–H···O(6)1# | O···O distance | 2.873(3) | 2.865(4) | 2.864(4) |
| hydrogen bond | O–H···O angle | 161.8 | 159.0 | 158.9 |
| O(7)–H···O(5)2# | O···O distance | 3.017(3) | 3.034(4) | 3.050(4) |
| hydrogen bond | O–H···O angle | 150.7 | 168.5 | 169.1 |
| [a]Symmetry transformations use to generate equivalent atoms (consistent with the symmetry transformations). (1#): $x + 1/2$, $y - 1/2$, $z + 1$; (2#): $x$, $-y + 1$, $z + 1/2$. | | | | |

**Table S2**. **Geometrical parameters of hydrogen bonds in 4 and 5**[a]

| Bond | | distance (Å) | |
|---|---|---|---|
| | | 4·Eu | 5·Gd |
| O(7)–H···O(1)1# | O···O distance | 2.709(4) | 2.701(4) |
| hydrogen bond | O–H···O angle | 147.3 | 160.7 |
| O(7)–H···O(5)2# | O···O distance | 2.779(5) | 2.789(5) |
| hydrogen bond | O–H···O angle | 138.1 | 159.1 |
| O(8)–H···O(5)3# | O···O distance | 2.778(5) | 2.785(5) |
| hydrogen bond | O–H···O angle | 168.9 | 155.5 |
| O(8)–H···O(6)4# | O···O distance | 2.740(4) | 2.735(5) |
| hydrogen bond | O–H···O angle | 144.0 | 162.7 |
| [a]Symmetry transformations use to generate equivalent atoms (consistent with the symmetry transformations). (1#): $x$, $y + 2$, $z + 1/2$; (2#): $x - 1/2$, $-y + 3/2$, $z + 1/2$; (3#): $x - 1/2$, $-y + 3/2$, $z - 1/2$; (4#): $x - 1/2$, $y + 1/2$, $z$. | | | |

**Table S3. Geometrical parameters of hydrogen bonds in 6–10**[a]

| bond | | distance (Å) | | | | |
|---|---|---|---|---|---|---|
| | | 6·Tb | 7·Dy | 8·Ho | 9·Er | 10·Lu |
| O(4)–H···O(3)1# distance | O···O | 2.711(3) | 2.709(4) | 2.591(3) | 2.715(3) | 2.725(3) |
| hydrogen bond | O–H···O angle | 176.1 | 168.2 | 166.7 | 176.1 | 164.6 |
| O(4)–H···O(1)2# distance | O···O | 2.589(3) | 2.581(4) | 2.717(3) | 2.577(3) | 2.572(3) |
| hydrogen bond | O–H···O angle | 157.8 | 153.7 | 167.5 | 158.9 | 150.6 |
| [a]Symmetry transformations use to generate equivalent atoms (consistent with the symmetry transformations). (1#): –x, –y, –z+1; (2#): $x - 1/2$, $-y + 1/2$, $-z + 1$. | | | | | | |




**Scheme S1.** The $hbpdcH_4$ ligand generated by an in situ ligand transformation reaction of demethylation of the $H_2mbpdc$ ligand during the hydrothermal reaction

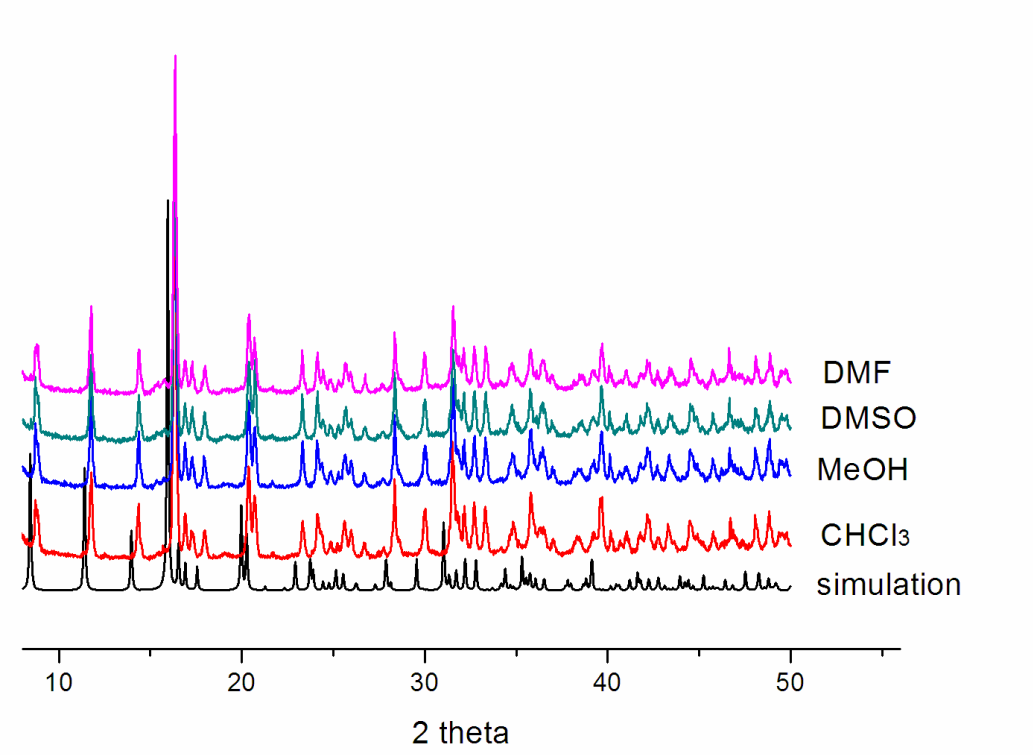



**Figure S1.** Comparison of the experimental powder patterns with the treatment of the different solvents with simulated powder pattern of polymer **10**.

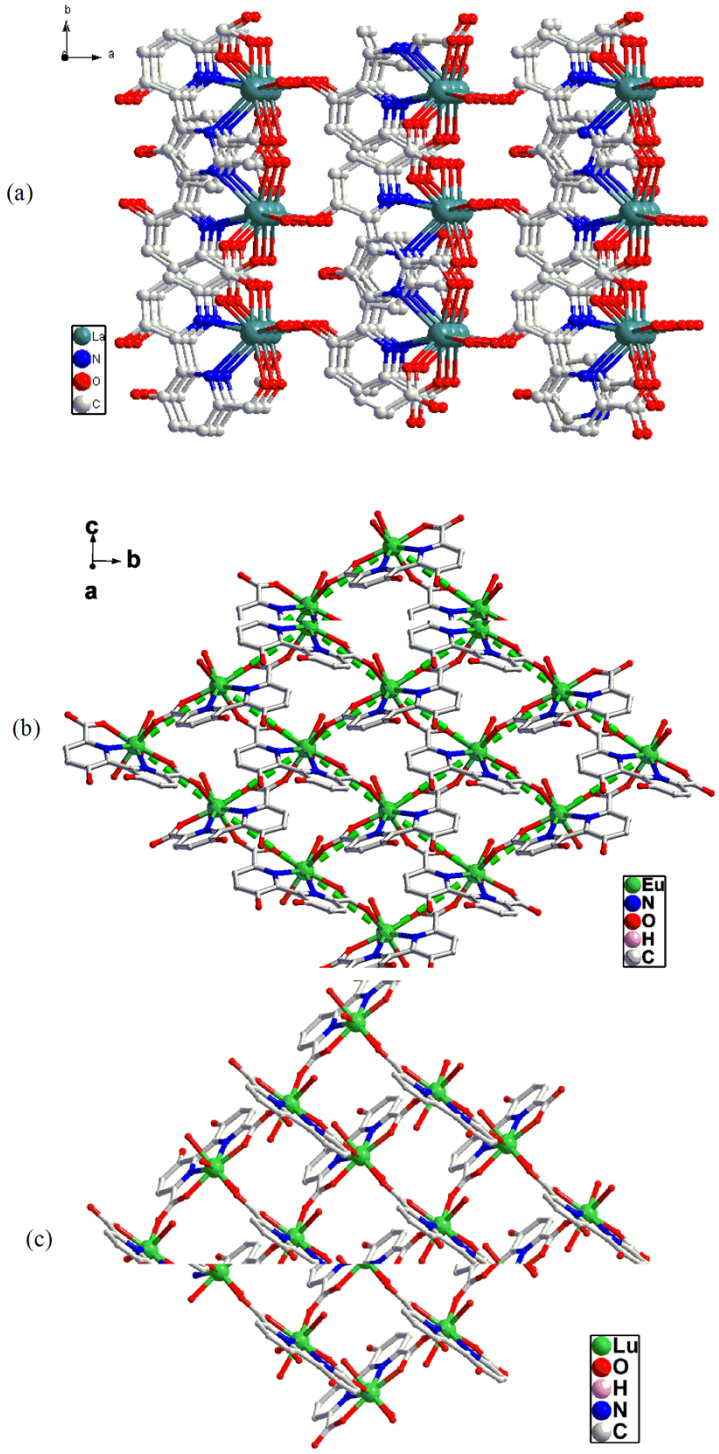



**Figure S2**. Side view of three different structures. (a) 3D structure for 1. (b) 2D $4^4$ grid for **4**. (c) 2D $4^4$ grid for **10**.

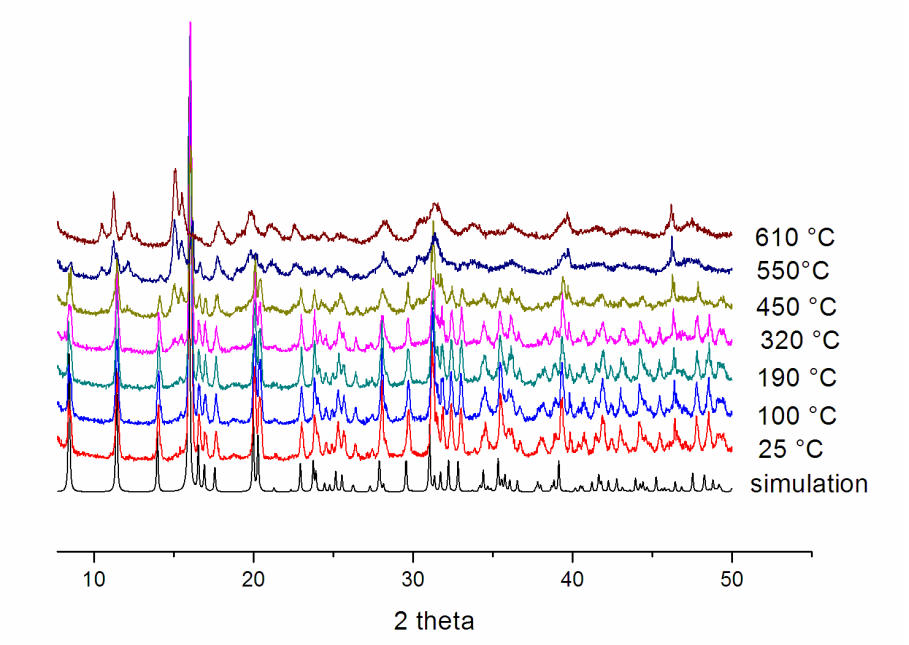



**Figure S3.** Comparison of the experimental powder patterns of the different temperature with simulated powder pattern of polymer **10**.