Electronic Supplementary Material (ESI) for CrystEngComm
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# Supplementary Information

**Table S1** Selected bond lengths (Å) and angles (°) for **1** and **2**

**Fig. S1** A polyhedral view illustrating the 2D layer structure of **1** ignoring the coordinated 3-Hpya molecules (color code: Cr, yellow; Mo, purple; Mn, green; Na, orange; O, red; N, blue; C, grey).

**Fig. S2** A polyhedral and ball-stick view illustrating the 3D supramolecular structure of **1** showing the π–π stacking interactions of 3-Hpya molecules along the *a* axis.

**Fig. S3** A polyhedral and ball-stick diagram of the 3D supramolecular framework structure of **2-α**, (color code: Cr, yellow; Mo, purple; Mn, green; O, red; N, blue; C, grey). Other atoms have been omitted for clarity.

**Fig. S4** A polyhedral and ball-stick diagram of the 3D supramolecular channel framework structure of **2-β**, (color code: Cr, yellow; Mo, purple; Mn, green; O, red; N, blue; C, grey). Free organic ligands and water molecules situated in the channels are omitted for clarity.

**Fig. S5** (a) IR spectrum for compound **1**. (b) IR spectrum for compound **2-α**. (c) IR spectrum for compound **2-β**.

**Fig. S6** UV-vis spectra for compounds **1, 2-α** and **2-β**.

**Fig. S7** (a) TG curve for compound **1**. (b) TG curve for compound **2-α**. (c) TG curve for compound **2-β**.

**Fig. S8** (a) The calculated and experimental PXRD patterns for compound **1.** (b) The calculated and experimental PXRD patterns for compound **2-α.** (c) The calculated and experimental PXRD patterns for compound **2-β.**

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**Table S1** Selected bond lengths (Å) and angles (°) for **1** and **2**

| | | | |
|---|---|---|---|
| Compound **1**[a] | | | |
| Mo(1)-O(7) | 1.698(3) | Cr(1)-O(1) | 1.959(2) |
| Mo(3)-O(12) | 1.720(3) | Cr(1)-O(3) | 1.977(2) |
| Mo(1)-O(8) | 1.731(3) | Mn(1)-O(13) | 2.170(3) |
| Mo(2)-O(9) | 1.703(3) | Mn(1)-OW1 | 2.174(3) |
| Mo(3)-O(11) | 1.710(3) | Mn(1)-O(8) | 2.215(3) |
| Mo(1)-O(4) | 1.894(3) | Na(1)-O(11) | 2.373(3) |
| Mo(2)-O(4) | 1.938(2) | Na(1)-O(9) | 2.336(3) |
| Mo(1)-O(3)#1 | 2.323(2) | Na(1)-O(16) | 2.764(3) |
| Mo(3)-O(1) | 2.245(2) | | |
| O(1)-Cr(1)-O(3)#1 | 84.54(1) | O(1)-Cr(1)-O(3) | 95.46(1) |
| O(2)#1-Cr(1)-O(2) | 180.000 | O(1)-Cr(1)-O(1)#1 | 180.000 |
| Compound **2-α** | | | |
| Mo(1)-O(13) | 1.687(3) | Cr(1)-O(2) | 1.966(3) |
| Mo(4)-O(19) | 1.713(3) | Cr(1)-O(4) | 1.988(3) |
| Mo(5)-O(22) | 1.715(3) | Mn(1)-OW3 | 2.182(4) |
| Mo(1)-O(14) | 1.727(3) | Mn(1)-OW2 | 2.129(4) |
| Mo(3)-O(8) | 1.909(3) | Mn(1)-O(27) | 2.051(4) |
| Mo(3)-O(9) | 1.979(3) | Mn(1)-O(25) | 2.177(4) |
| Mo(5)-O(4) | 2.236(3) | Mn(2)-OW4 | 2.213(4) |
| Mo(5)-O(5) | 2.344(3) | Mn(2)-OW5 | 2.133(4) |
| | | Mn(2)-O(14) | 2.179(3) |
| O(1)-Cr(1)-O(6) | 83.77(1) | O(3)-Cr(1)-O(1) | 96.51(1) |
| O(1)-Cr(1)-O(4) | 178.29(1) | O(3)-Cr(1)-O(6) | 179.22(1) |
| Compound **2-β**[b] | | | |
| Mo(1)-O(7) | 1.685(3) | Cr(1)-O(2) | 1.951(4) |
| Mo(4)-O(19) | 1.712(4) | Cr(1)-O(3) | 1.979(4) |
| Mo(1)-O(8) | 1.739(4) | Mn(1)-O(9) | 2.222(5) |
| Mo(2)-O(9) | 1.740(4) | Mn(1)-O(8) | 2.250(4) |
| Mo(2)-O(5) | 1.905(3) | Mn(1)-O(25) | 2.186(5) |
| Mo(3)-O(6) | 1.958(4) | Mn(1)-OW1 | 2.144(4) |
| Mo(1)-O(1) | 2.256(4) | Mn(1)-OW3 | 2.225(4) |
| Mo(4)-O(14) | 2.371(3) | Mn(2)-O(27) | 2.107(5) |
| Mn(2)-OW4 | 2.232(4) | Mn(2)-OW5 | 2.197(4) |
| O(2)-Cr(1)-O(1) | 83.99(1) | O(2)-Cr(1)-O(1)#2 | 96.01(1) |
| O(2)#2-Cr(1)-O(2) | 180.00 | O(14)-Cr(2)-O(14)#3 | 180.000 |

[a]Symmetry transformations used to generate equivalent atoms: #1 -x,-y+4,-z+2 #2 -x,-y+3,-z+1 #3 -x+1,-y+4,-z+2

[b]Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1 #2 -x+1,-y+1,-z #3 -x,-y+1,-z+1

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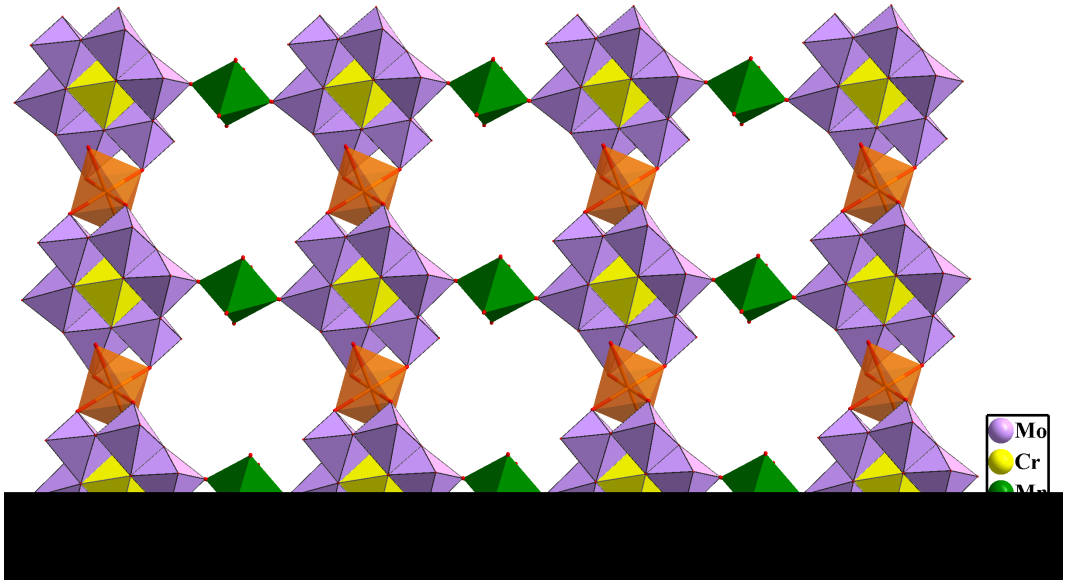


**Fig. S1**

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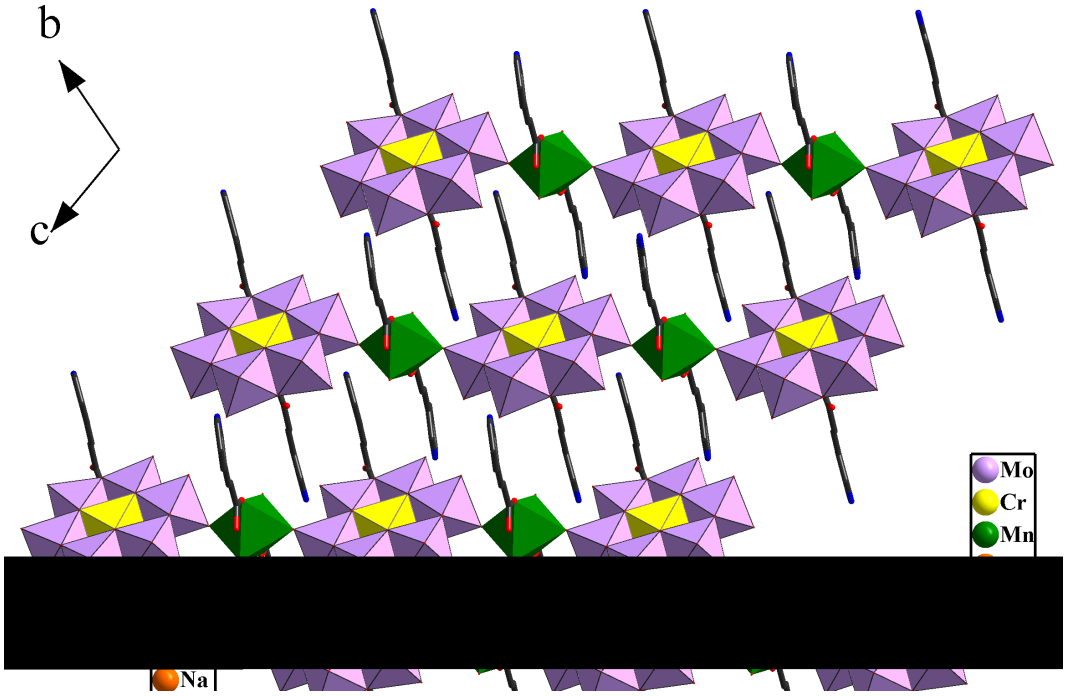


**Fig. S2**

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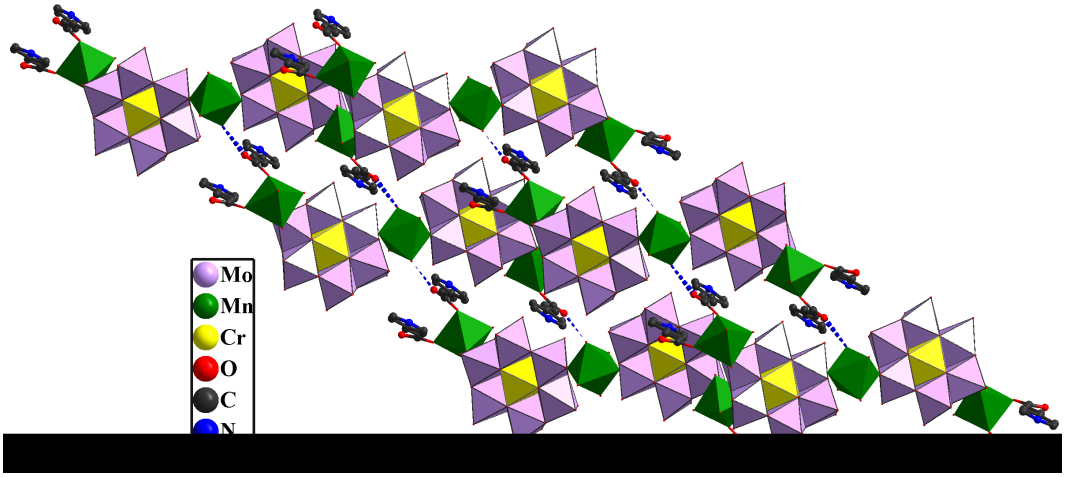


**Fig. S3**

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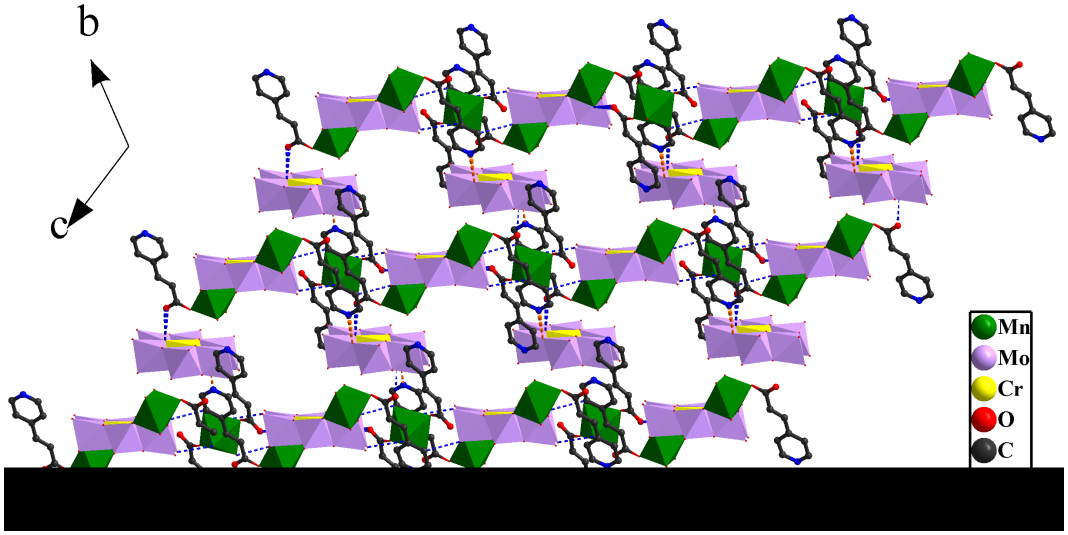


**Fig. S4**

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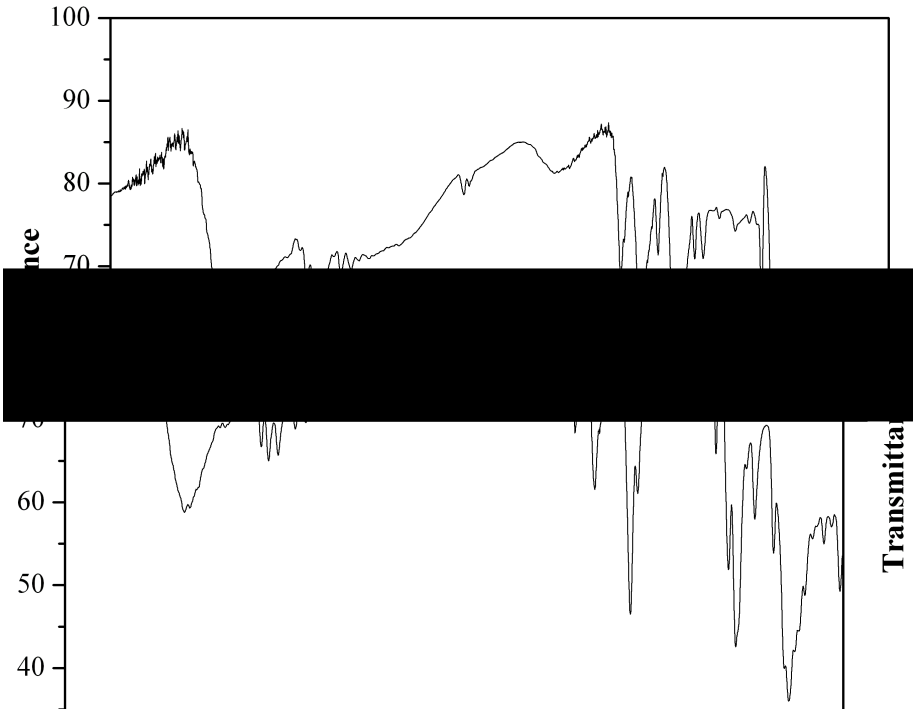


**Fig. S5a**

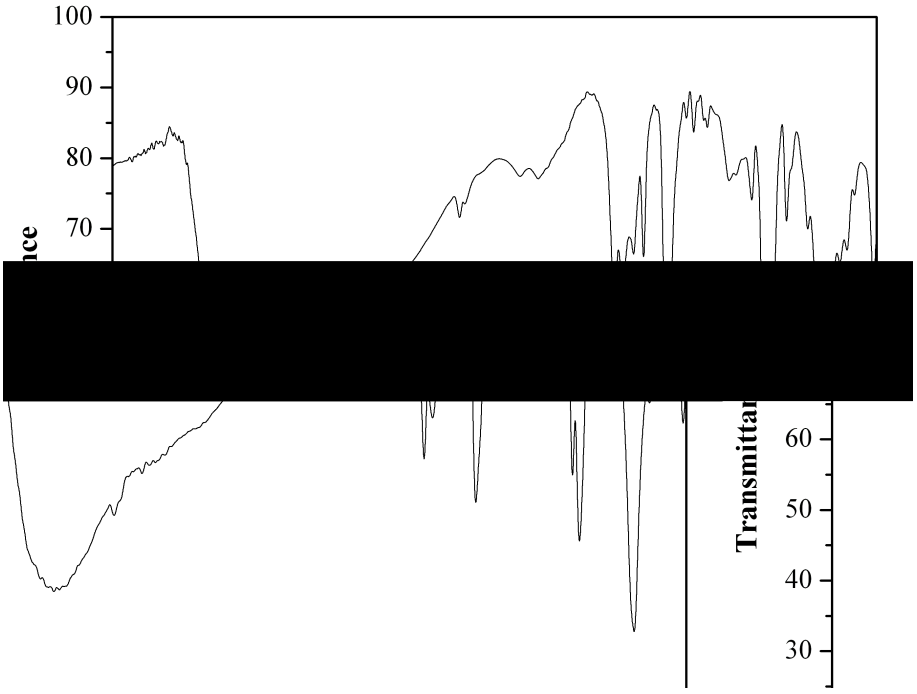


**Fig. S5b**

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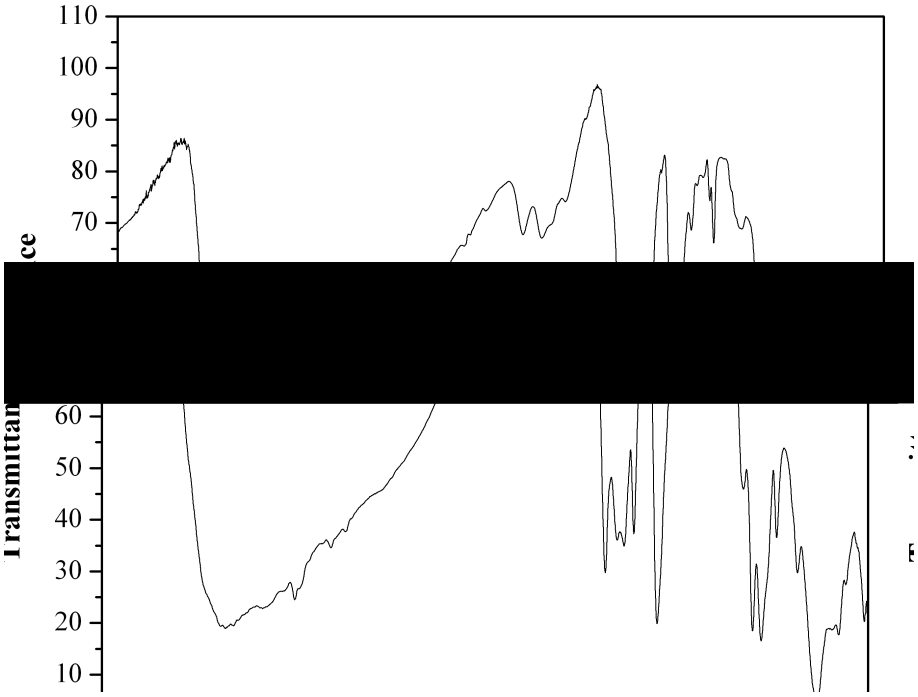


**Fig. S5c**

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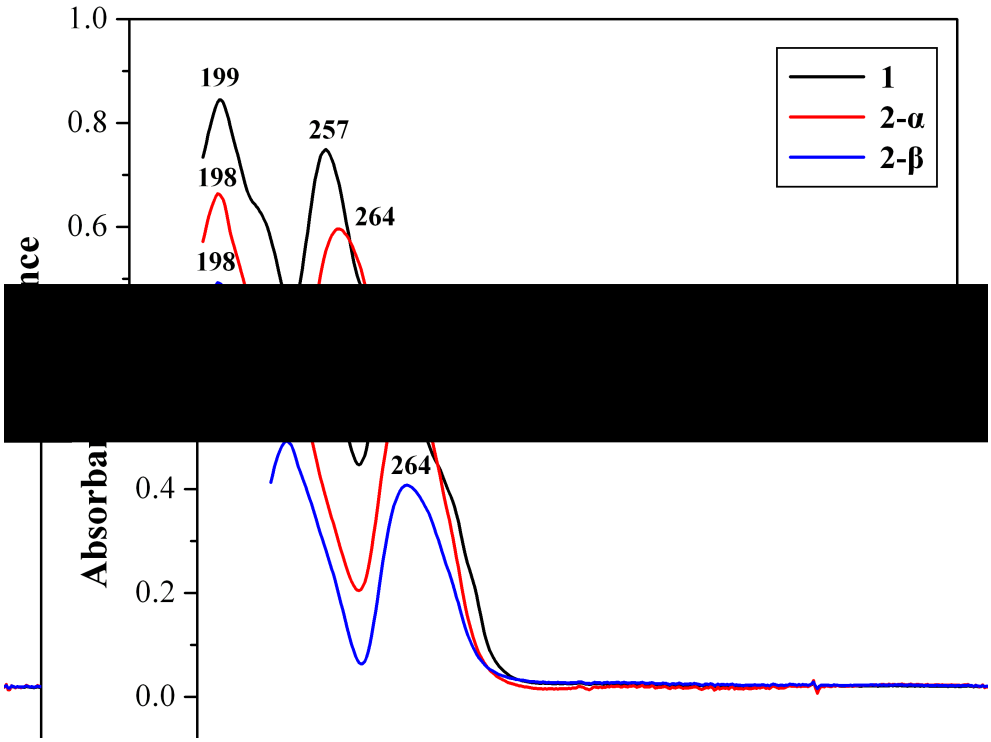


**Fig. S6**

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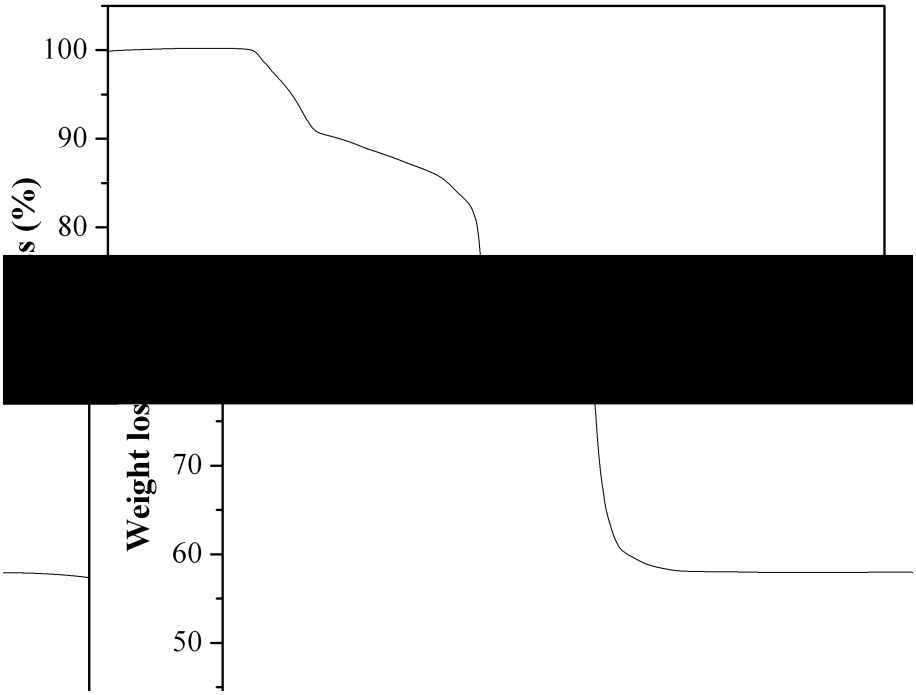


**Fig. S7a**

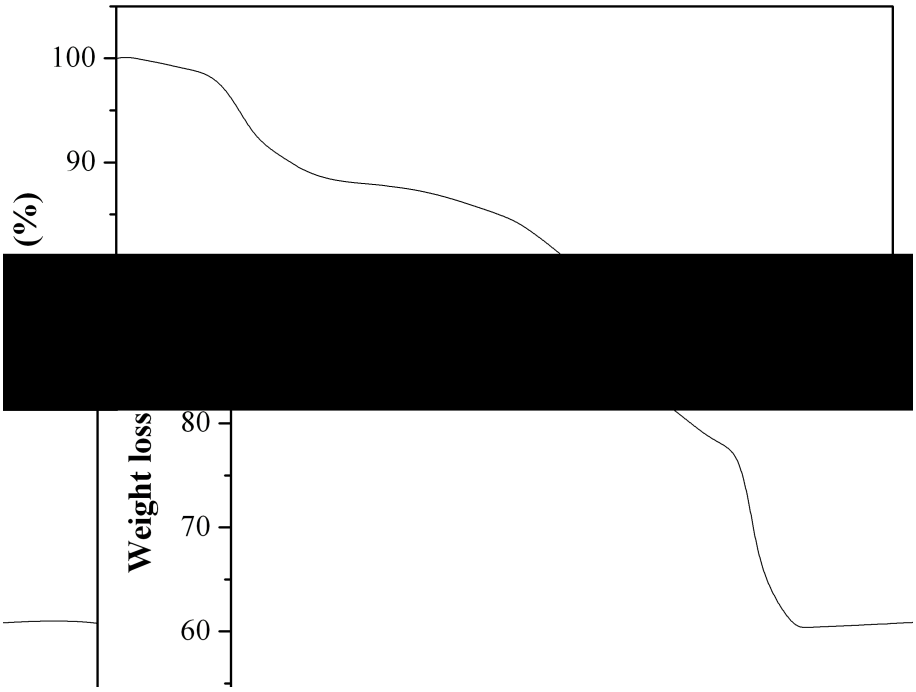


**Fig. S7b**

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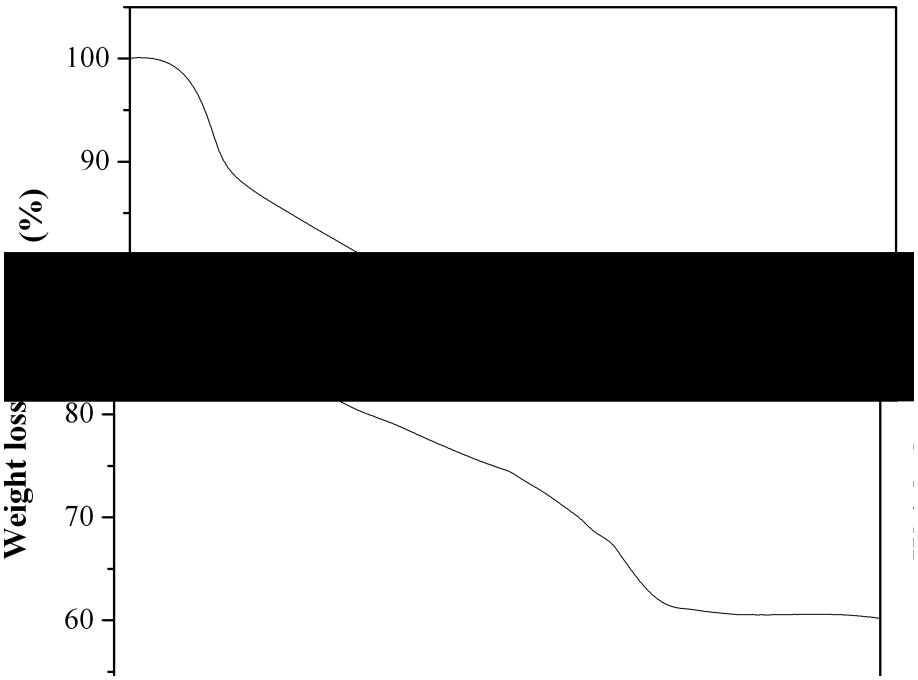


**Fig. S7c**

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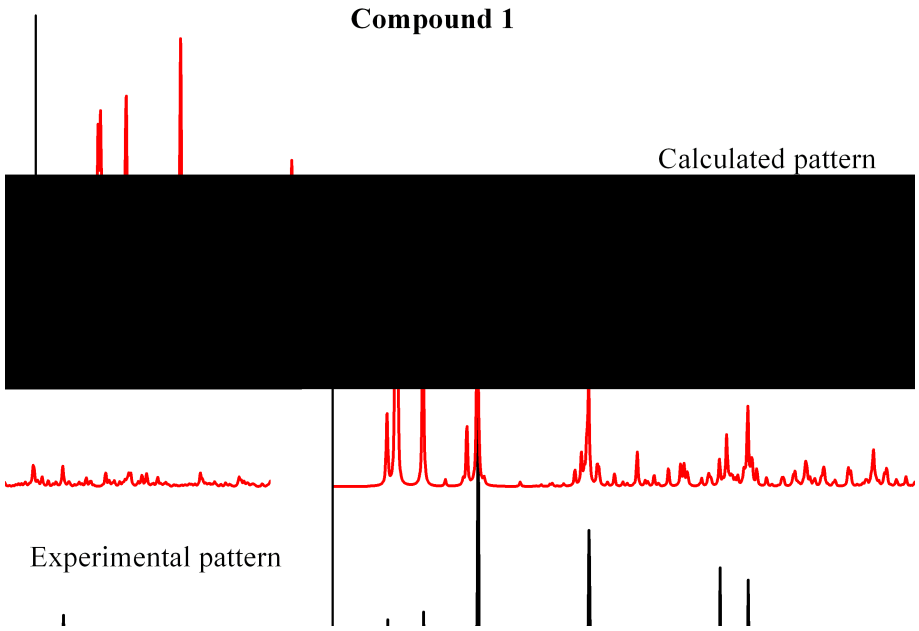


**Fig. S8a**

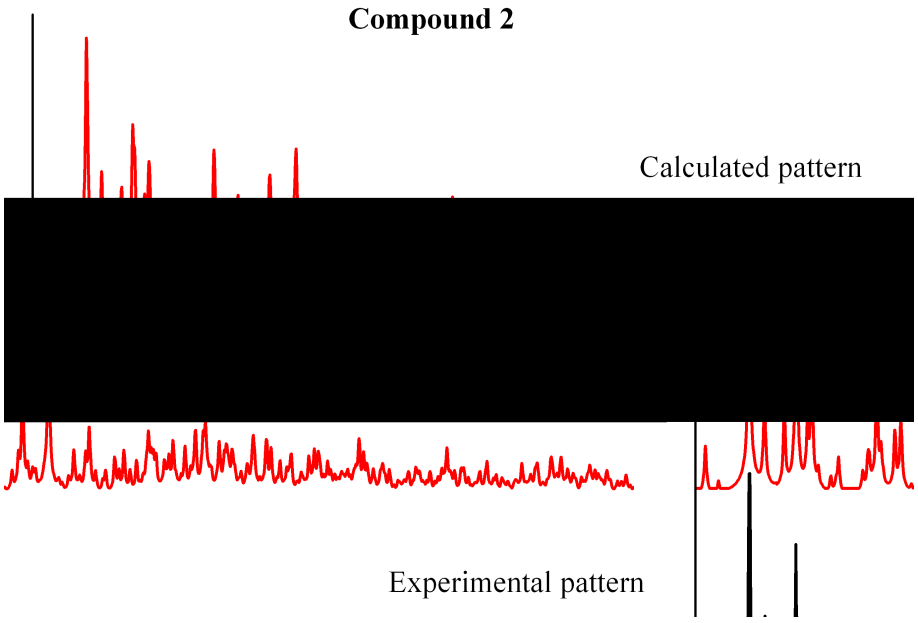


**Fig. S8b**

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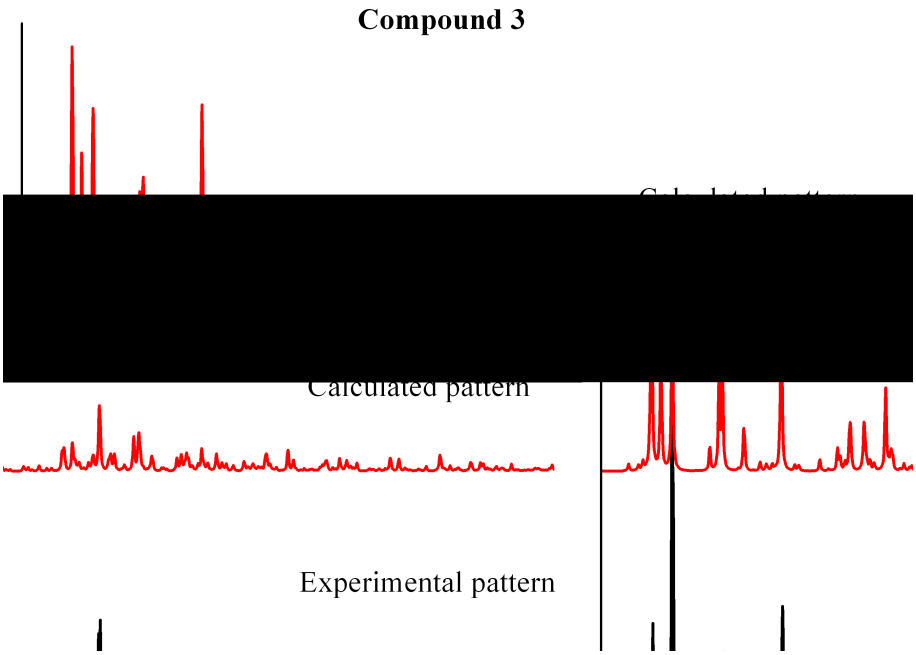


**Fig.S8c**