# *Electronic supplementary information (ESI)*

# Structural diversity in imidazole and carboxylate-containing metal complexes dependent on the alkaline reagents

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**Table S1** Selected bond lengths (Å) and bond angles (°) for complexes **1** - **5**

**1**

| | | | |
|---|---|---|---|
| Cd(1)-O(6) | 2.283(3) | Cd(1)-N(12)#1 | 2.292(3) |
| Cd(1)-O(5) | 2.295(3) | Cd(1)-O(1) | 2.305(2) |
| Cd(1)-O(4)#2 | 2.347(2) | Cd(1)-O(2) | 2.542(2) |
| Cd(1)-O(3)#2 | 2.588(3) | | |
| O(6)-Cd(1)-N(12)#1 | 169.48(9) | O(6)-Cd(1)-O(5) | 77.65(11) |
| N(12)#1–Cd(1)–O(5) | 91.88(11) | O(6)-Cd(1)-O(1) | 92.84(10) |
| N(12)#1–Cd(1)–O(1) | 95.01(10) | O(6)-Cd(1)-O(4)#2 | 96.69(10) |
| N(12)#1–Cd(1)–O(4)#2 | 91.29(10) | O(1)-Cd(1)-O(4)#2 | 82.33(8) |
| O(6)–Cd(1)–O(2) | 90.96(10) | N(12)#1-Cd(1)-O(2) | 88.12(9 ) |
| O(5)–Cd(1)–O(2) | 92.01(9) | O(1)-Cd(1)-O(2) | 53.45(7) |
| O(6)–Cd(1)–O(3)#2 | 87.80(10) | N(12)#1-Cd(1)-O(3)#2 | 91.71(10) |
| O(5)-Cd(1)-O(3)#2 | 80.23(9) | O(4)#2-Cd(1)-O(3)#2 | 52.29(8) |

**2**

| | | | |
|---|---|---|---|
| Cd(1)-N(12)#1 | 2.241(3) | Cd(1)-O(1) | 2.291(3) |
| Cd(1)-O(5) | 2.315(3) | Cd(1)-O(4)#2 | 2.349(3) |
| Cd(1)-O(6) | 2.369(4) | Cd(1)-O(3)#2 | 2.543(3) |
| Cd(1)-O(2) | 2.636(3) | | |
| N(12)#1-Cd(1)-O(5) | 93.35(12) | O(1)-Cd(1)-O(5) | 90.14(11) |
| O(1)-Cd(1)-O(4)#2 | 84.48(10) | O(5)-Cd(1)-O(4)#2 | 88.07(11) |
| N(12)#1-Cd(1)-O(6) | 91.26(13) | O(1)-Cd(1)-O(6) | 87.30(13) |
| O(5)-Cd(1)-O(6) | 175.24(11) | O(4)#2-Cd(1)-O(6) | 87.69(12) |
| N(12)#1-Cd(1)-O(3)#2 | 85.38(11) | O(5)-Cd(1)-O(3)#2 | 84.10(11) |
| O(4)#2-Cd(1)-O(3)#2 | 53.43(10) | O(6)-Cd(1)-O(3)#2 | 95.10(13) |
| N(12)#1-Cd(1)-O(2) | 85.26(10) | O(1)-Cd(1)-O(2) | 52.12(9) |
| O(5)-Cd(1)-O(2) | 101.27(11) | O(6)-Cd(1)-O(2) | 80.29(13) |

**3**

| | | | |
|---|---|---|---|
| Cd(1)-N(111) | 2.262(4) | Cd(1)-O(4)#1 | 2.278(3) |
| Cd(1)-O(3)#2 | 2.301(3) | Cd(1)-O(9) | 2.319(3) |
| Cd(1)-O(2) | 2.323(3) | Cd(1)-O(1) | 2.538(4) |
| Cd(2)-N(12)#3 | 2.234(4) | Cd(2)-O(8)#4 | 2.247(4) |
| Cd(2)-O(7) | 2.254(4) | Cd(2)-O(10) | 2.361(4) |
| Cd(2)-O(5)#1 | 2.370(3) | Cd(2)-O(6)#1 | 2.396(4) |
| N(111)-Cd(1)-O(4)#1 | 114.63(14) | N(111)-Cd(1)-O(3)#2 | 93.41(14) |
| O(4)#1-Cd(1)-O(3)#2 | 101.06(12) | N(111)-Cd(1)-O(9) | 85.42(14) |
| O(4)#1-Cd(1)-O(9) | 86.96(12) | O(3)#2-Cd(1)-O(9) | 171.59(12) |
| N(111)-Cd(1)-O(2) | 110.36(14) | O(3)#2-Cd(1)-O(2) | 89.35(13) |
| O(9)-Cd(1)-O(2) | 83.28(13) | O(4)#1-Cd(1)-O(1) | 80.40(13) |
| O(3)#2-Cd(1)-O(1) | 89.67(13) | O(9)-Cd(1)-O(1) | 89.20(12) |
| O(2)-Cd(1)-O(1) | 53.57(12) | N(12)#3-Cd(2)-O(8)#4 | 90.70(15) |
| N(12)#3-Cd(2)-O(7) | 96.00(17) | O(8)#4-Cd(2)-O(7) | 121.97(14) |
| N(12)#3-Cd(2)-O(10) | 177.34(15) | O(8)#4-Cd(2)-O(10) | 87.70(14) |
| O(7)-Cd(2)-O(10) | 83.07(16) | N(12)#3-Cd(2)-O(5)#1 | 94.52(14) |
| O(7)-Cd(2)-O(5)#1 | 86.18(14) | O(10)-Cd(2)-O(5)#1 | 87.91(12) |
| N(12)#3-Cd(2)-O(6)#1 | 87.79(15) | O(8)#4-Cd(2)-O(6)#1 | 96.47(13) |
| O(10)-Cd(2)-O(6)#1 | 94.49(14) | O(5)#1-Cd(2)-O(6)#1 | 55.03(12) |

**4**

| | | | |
|---|---|---|---|
| Zn(1)-O(3)#1 | 1.9504(14) | Zn(1)-O(1) | 1.9815(16) |
| Zn(1)-O(4)#2 | 1.9878(14) | Zn(1)-N(12)#3 | 1.9965(18) |
| O(3)#1-Zn(1)-O(1) | 114.01(7) | O(3)#1-Zn(1)-O(4)#2 | 109.49(6) |
| O(1)-Zn(1)-O(4)#2 | 104.93(6) | O(3)#1-Zn(1)-N(12)#3 | 116.71(7) |
| O(1)-Zn(1)-N(12)#3 | 114.19(7) | O(4)#2-Zn(1)-N(12)#3 | 94.90(7) |
| **5** | | | |
| Zn(1)-O(2)#1 | 1.9152(15) | Zn(1)-O(3)#2 | 1.9624(14) |
| Zn(1)-N(12) | 1.9650(18) | Zn(1)-O(5) | 2.0060(14) |
| O(2)#1-Zn(1)-O(3)#2 | 96.87(6) | O(2)#1-Zn(1)-N(12) | 125.21(7) |
| O(3)#2-Zn(1)-N(12) | 115.59(7) | O(2)#1-Zn(1)-O(5) | 106.93(6) |
| O(3)#2-Zn(1)-O(5) | 108.50(6) | N(12)-Zn(1)-O(5) | 102.95(7) |

Symmetry transformations used to generate equivalent atoms:

For **1**, #1 2-x, 2-y, 2-z; #2 x, -1+y, z; for **2**, #1 1/2-x, 1/2+y, 1/2-z; #2 1+x, y, z; for **3**, #1 x, -1+y, z; #2 -x, 1-y, 1-z; #3, 1+x, -1+y, 1+z; #4 2-x, -y, 2-z; for **4**, #1 3/2-x, -1/2+y, 1/2-z; #2 -1/2+x, 1/2-y, -1/2+z; #3 1-x, 1-y, -z; for **5**, #1 1-x, -1/2+y, 1/2-z; #2 1/2-x, 1-y, -1/2+z.

**Table S2**. Hydrogen bonding data for complexes **1** and **2.**

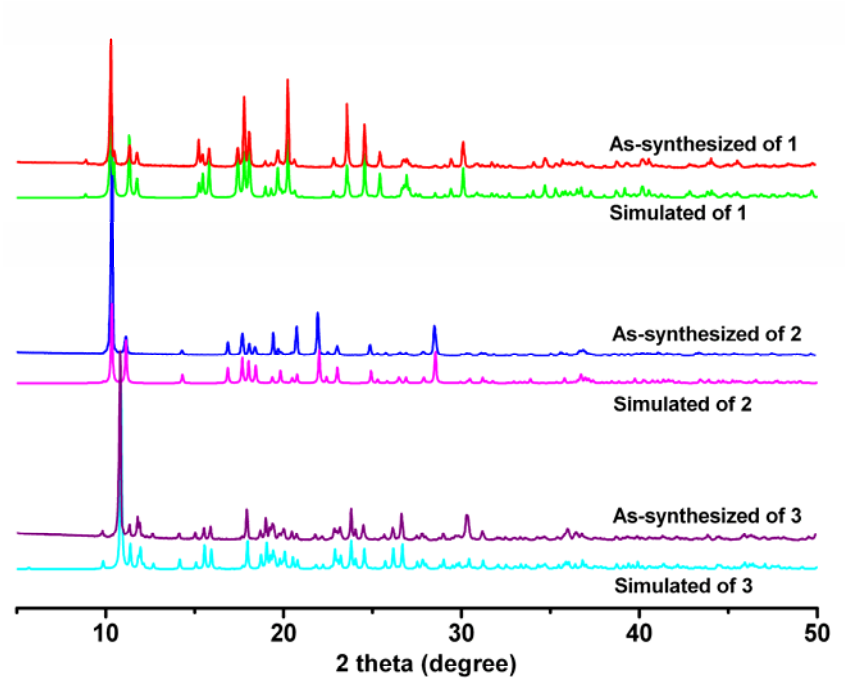
| D-H···A | d(D···A) (Å) | ∠D-H···A (°) |
|---|---|---|
| Complex **1** | | |
| O(5)-H(17)···O(7)#1 | 2.947(5) | 158 |
| O(5)-H(16)···O(2)#2 | 2.650(4) | 174 |
| O(7)-H(18)···O(3) | 2.791(5) | 163 |
| O(7)-H(19)···O3#3 | 2.898(5) | 134 |
| Complex **2** | | |
| O(6)-H(12)···O(1)#1 | 2.765(5) | 169 |
| O(5)-H(10)···O(3)#2 | 2.749(4) | 155 |

Symmetry transformations used to generate equivalent atoms: for **1**, #1 x, y-1, z; #2 -x+1, -y+1, -z+1; #3 -x+1, -y+2, -z+1; for **2**, #1 -x+1, -y+2, -z+1; #2 -x, -y+2, -z.

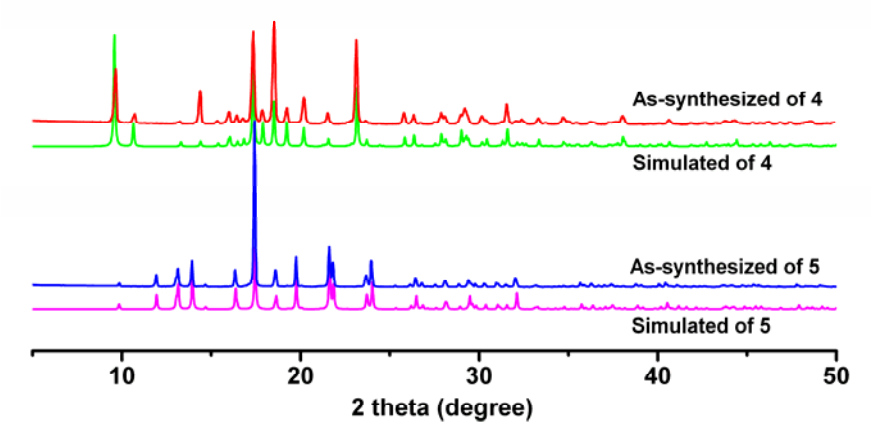
**Table S3**. Torsion angles and dihedral angles of $L^{2-}$ ligands in complexes **1** - **5**.

| Complex | Torsion angle (°) | | | | Dihedral angle (°) [a] |
|---|---|---|---|---|---|
| **1** | N11-C11-C1-C2 | 65.4(4) | N11-C11-C1-C6 | -116.3(3) | 85.7 |
| **2** | N11-C11-C1-C2 | -47.3(5) | N11-C11-C1-C6 | 133.4(4) | 78.7 |
| **3** | N11-C11-C1-C2 | -138.9(5) | N11-C11-C1-C6 | 40.0(7) | 89.2 |
| | N112-C111-C101-C102 | 167.7(5) | N112-C111-C101-C106 | -16.2(8) | 62.4 |
| **4** | N11-C11-C1-C2 | -50.4(3) | N11-C11-C1-C6 | 129.3(2) | 81.2 |
| **5** | N11-C11-C1-C2 | 25.0(3) | N11-C11-C1-C6 | -154.4(2) | 72.4 |

[a] The dihedral angle between the central benzene ring plane and imidazole ring plane in $L^{2-}$ ligand.

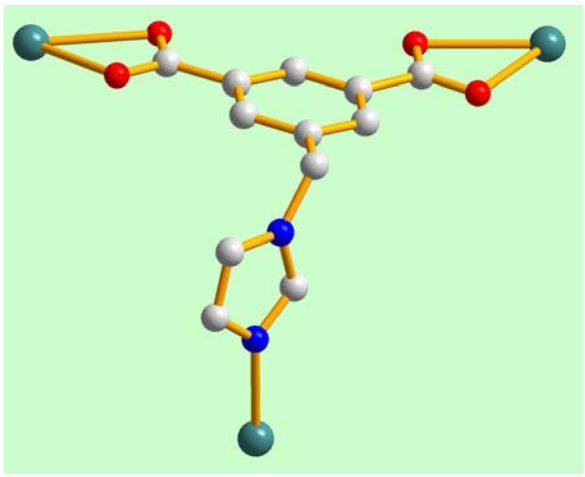



(a)

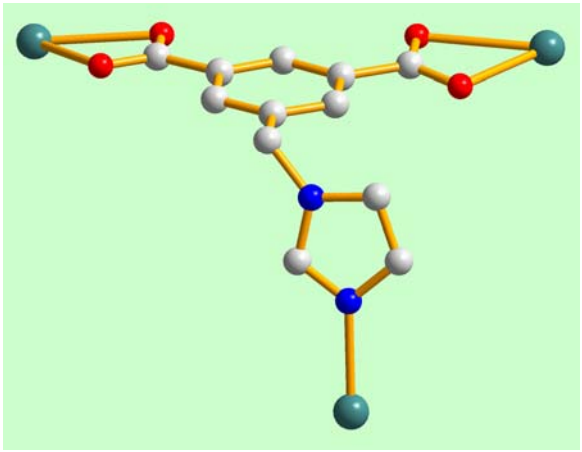



(b)

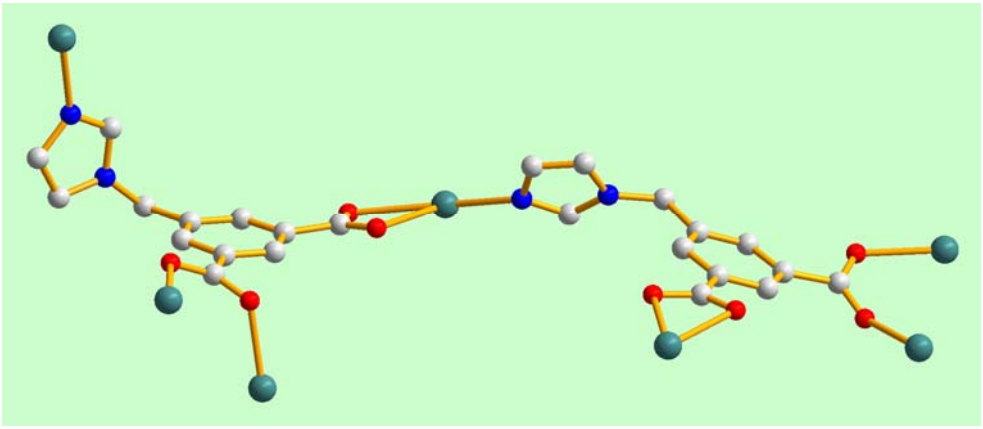
**Figure S1.** The powder X-ray diffractions (PXRD) patterns: **(**a) complexes **1** - **3**; (b) complexes **4** - **5**.



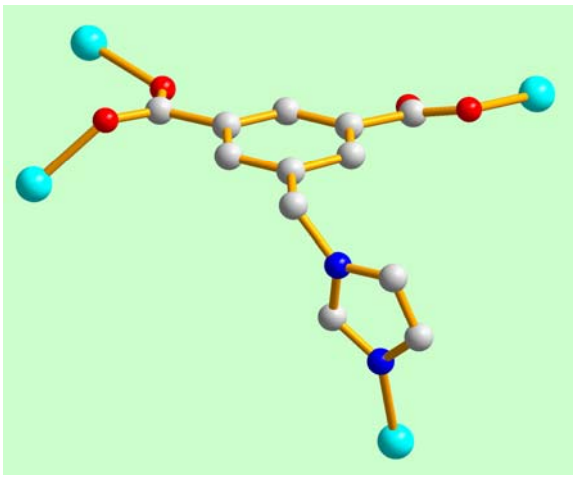
(a) Complex **1**



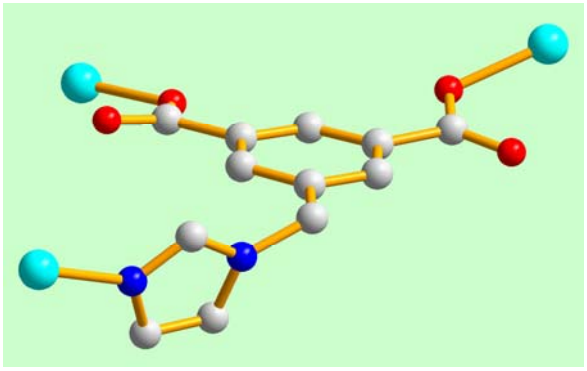
(b) Complex **2**



(c) Complex **3**



(e) Complex **4**



(f) Complex **5**

**Figure S2.** The molecular conformations of $L^{2-}$ ligands appeared in complexes **1** - **5**.

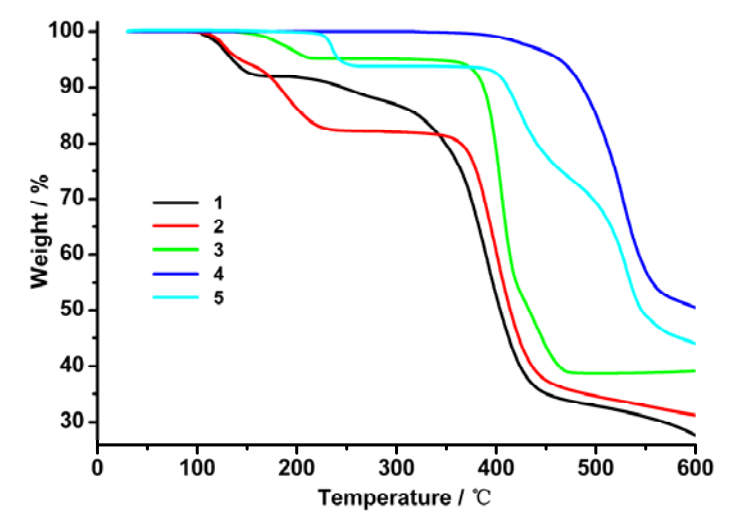



**Figure S3**. The TGA curves of complexes **1 - 5**.

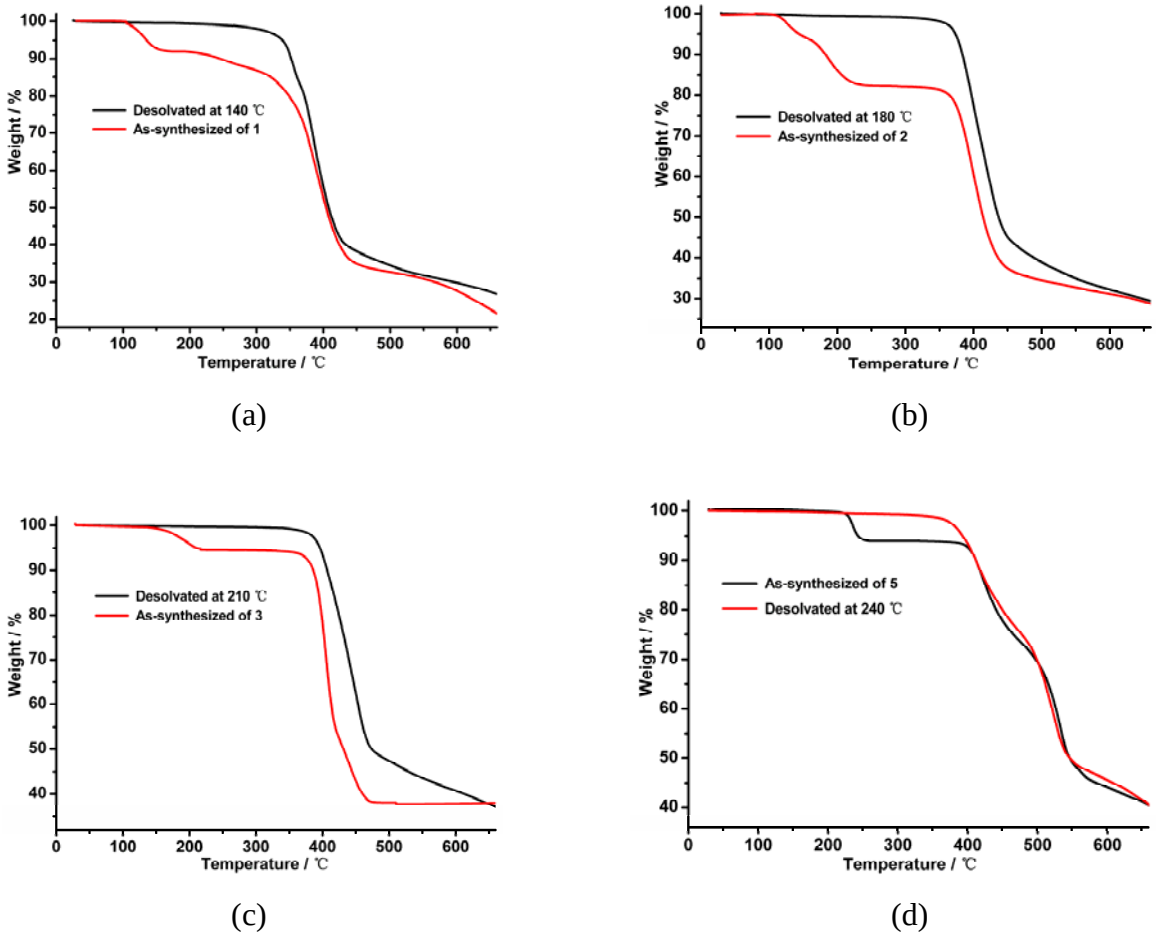



**Figure S4**. The TGA curves of the desolvated samples: **1** (a), **2** (b), **3** (c), and **5** (d).

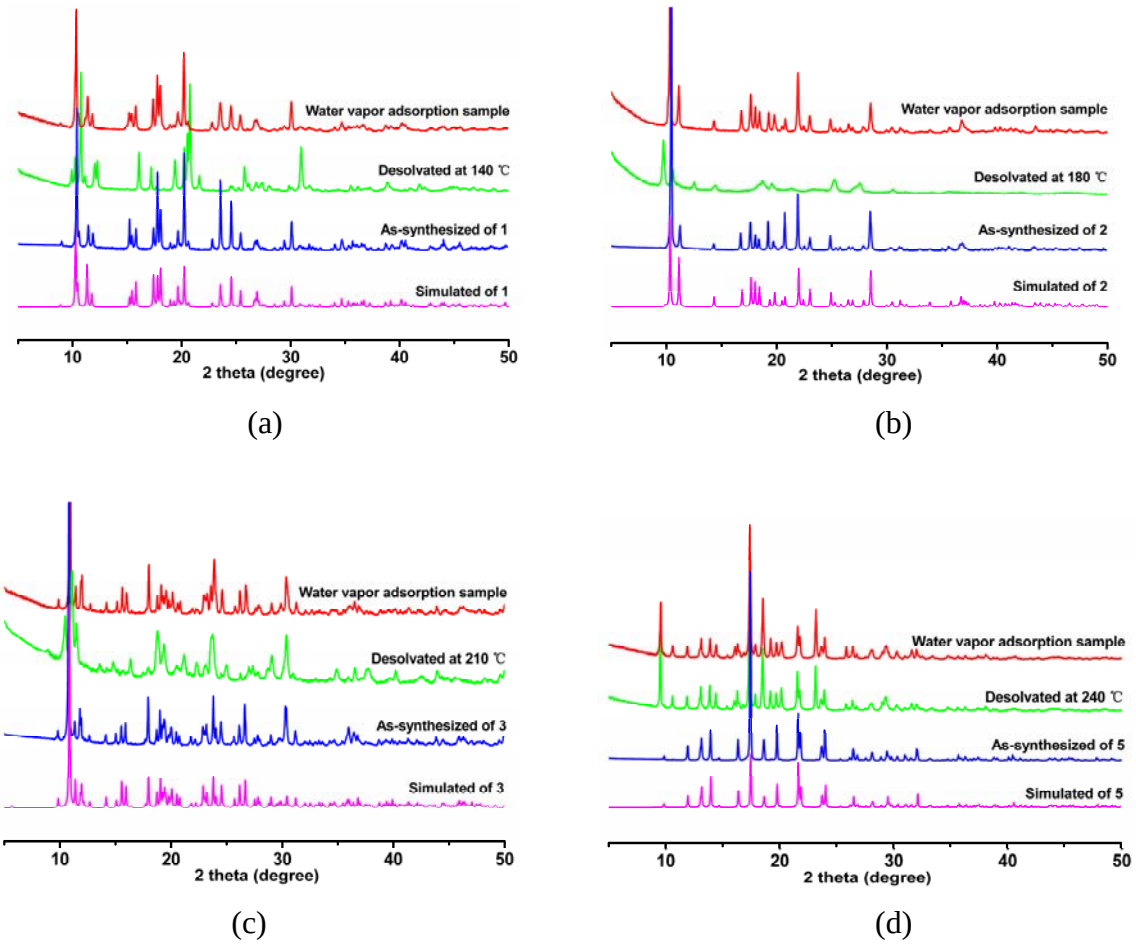



**Figure S5**. The powder X-ray diffractions (PXRD) patterns of the dehydrated and rehydrated samples: **1** (a), **2** (b), **3** (c), and **5** (d).