Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Temperature-induced racemic compounds and chiral conglomerates based on polyoxometalates and lanthanides: syntheses, structures and catalytic properties

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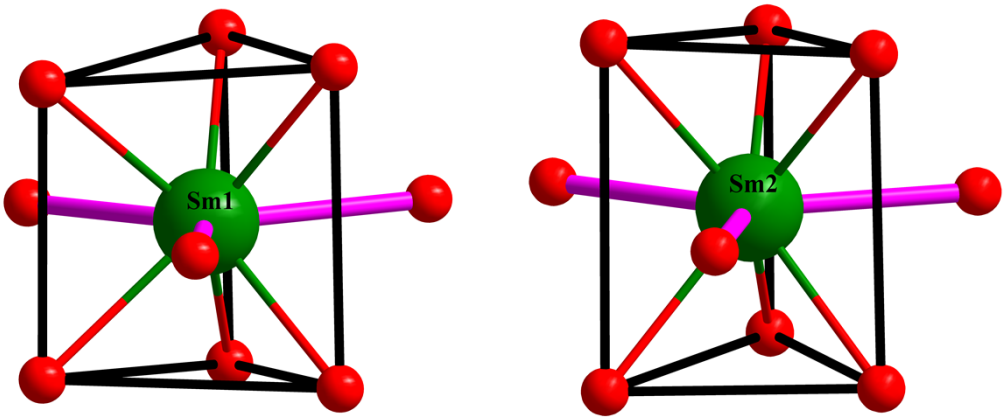

Fig. S1 Ball-stick representation of the tricapped trigonal prism coordination modes of Sm(1) and Sm(2) cations in **1**.

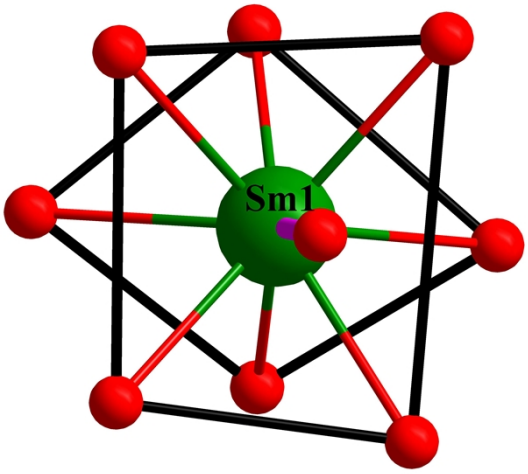

Fig. S2 Ball-stick representation of the monocapped square antiprismatic coordination mode of Sm(1) cation in **3**.

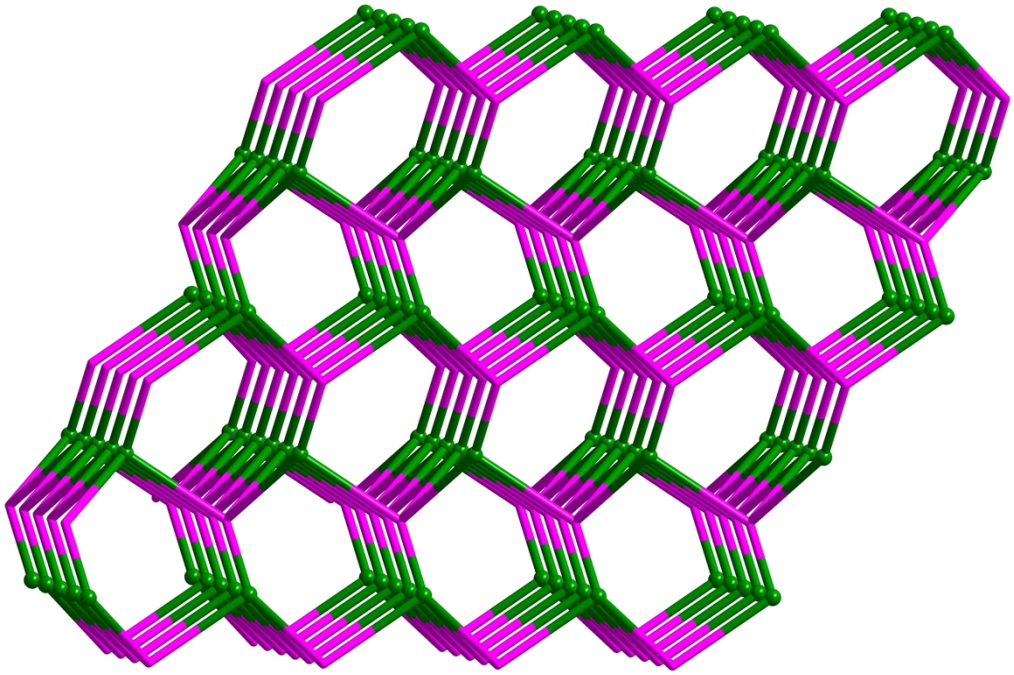

Fig. S3 Schematic representation of the 4-connected diamond topology of **3**.

II. Supplementary Physical Characterizations

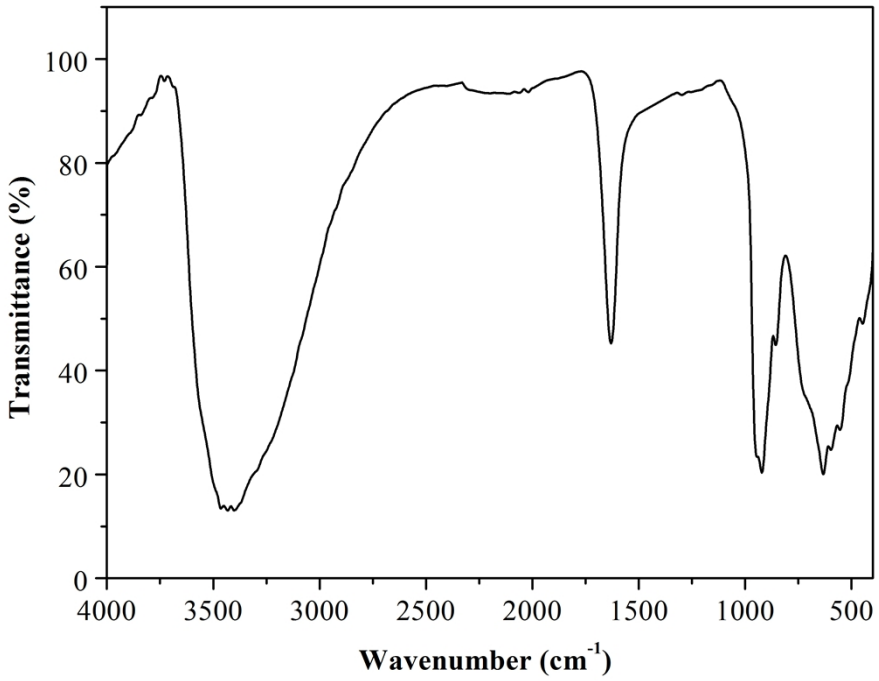

Fig. S4a IR spectrum for compound **1**.

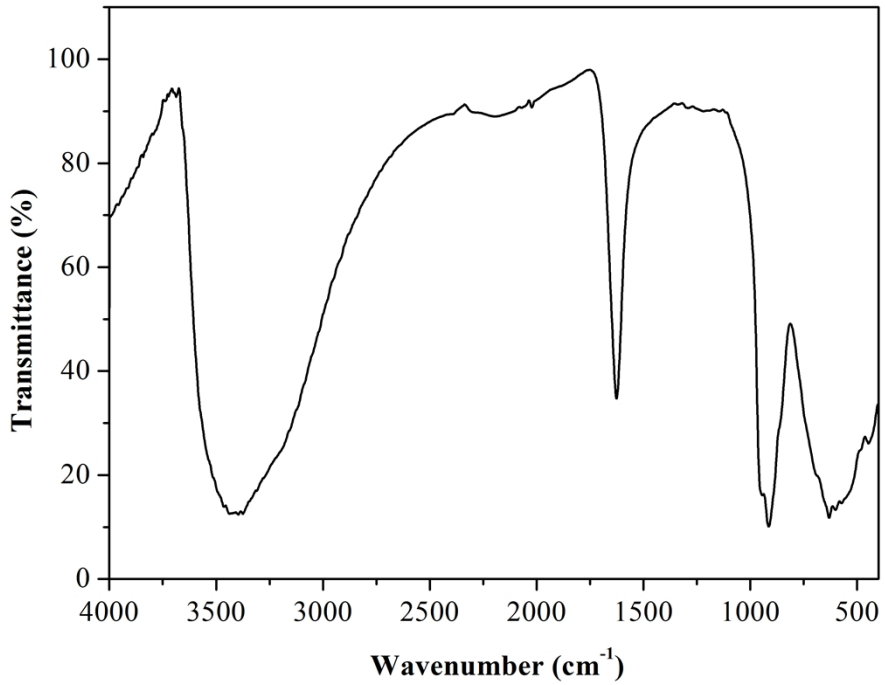

Fig. S4b IR spectrum for compound **2**.

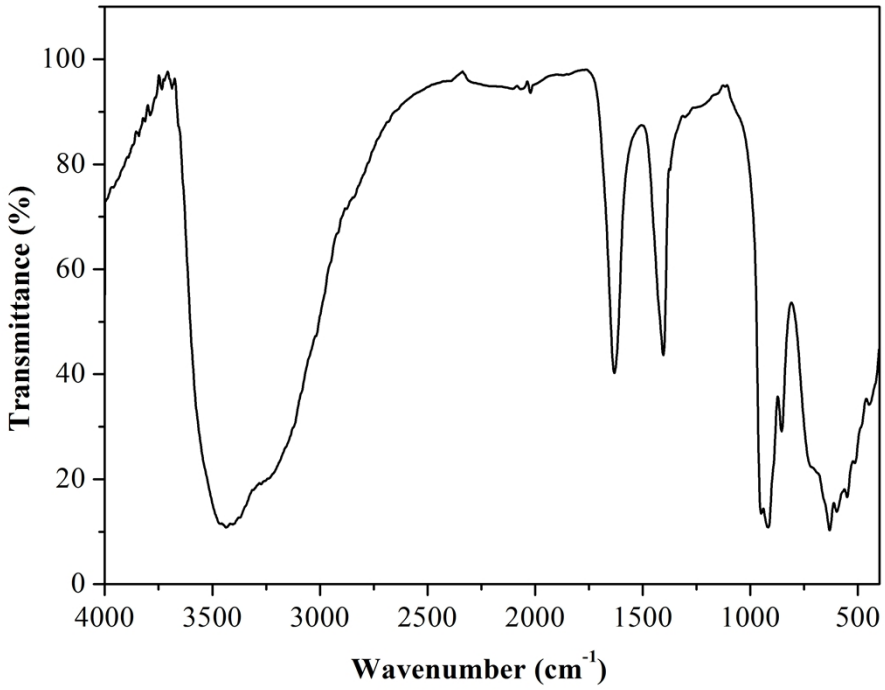

Fig. S4c IR spectrum for compound **3**.

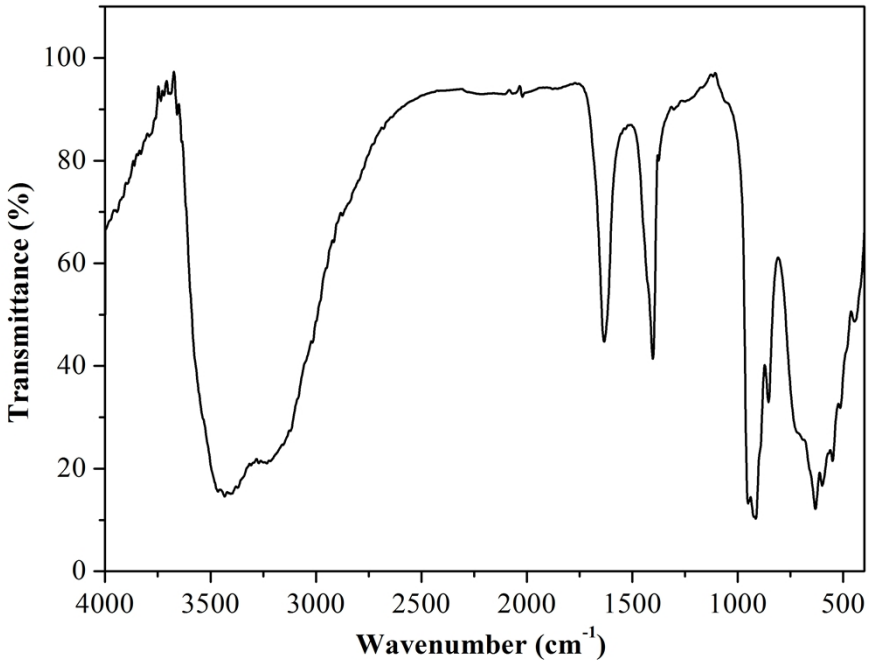

Fig. S4d IR spectrum for compound **4**.

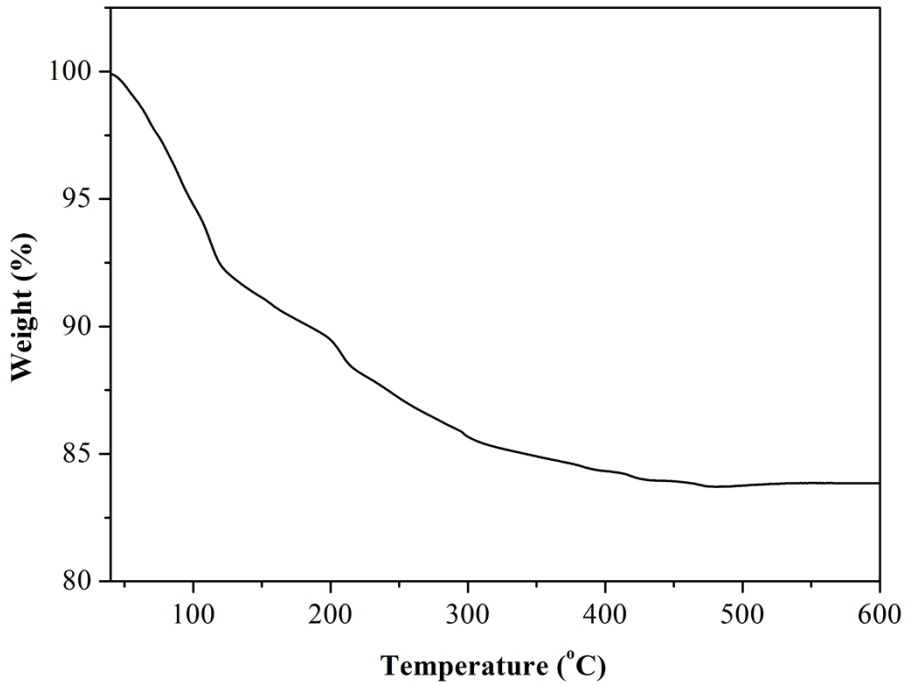

Fig. S5a TG curve for compound **1**.

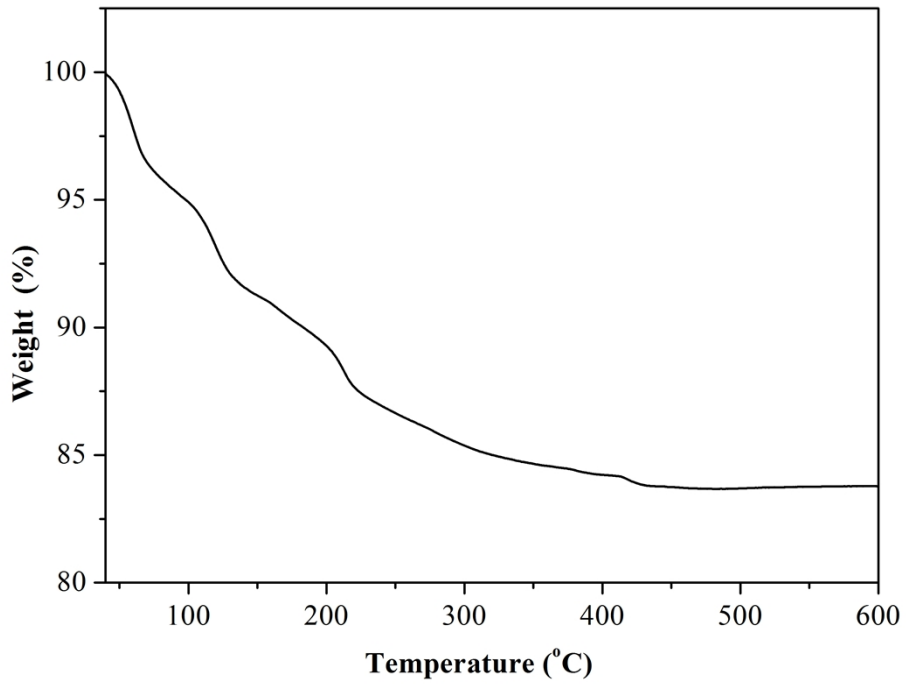

Fig. S5b TG curve for compound **2**.

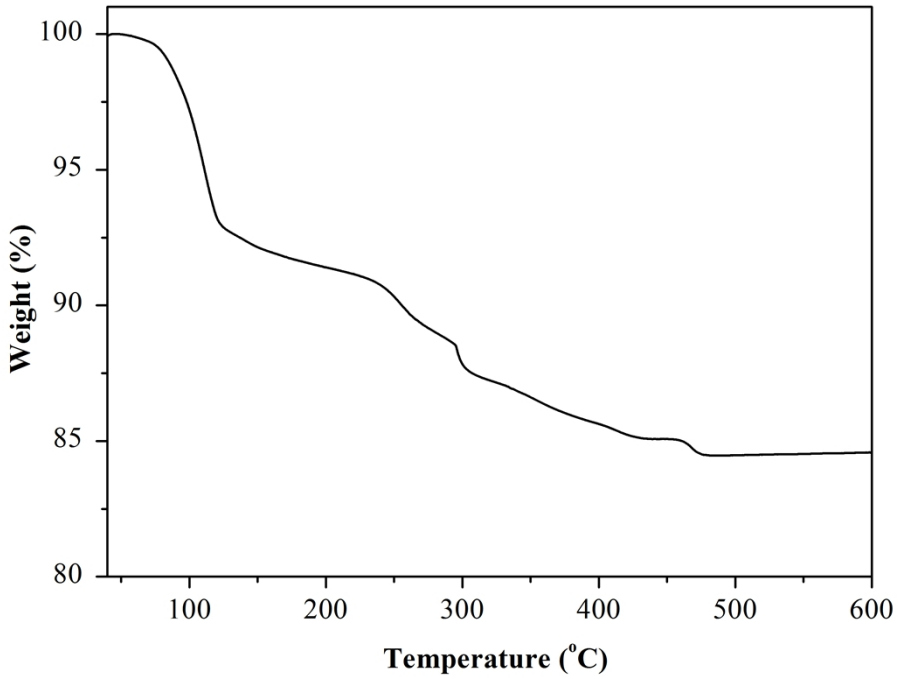

Fig. S5c TG curve for compound **3**.

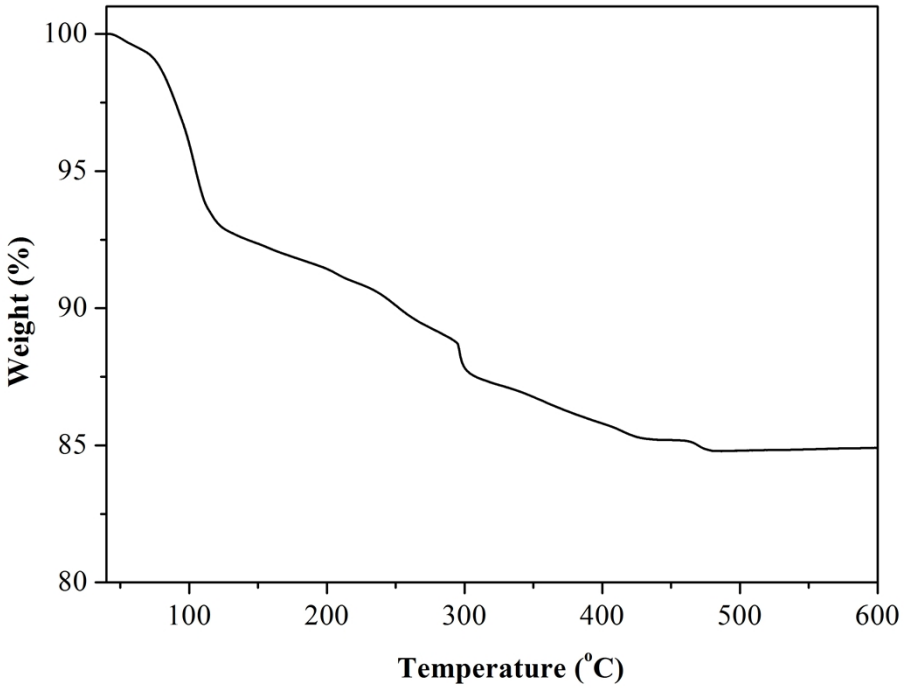

Fig. S5d TG curve for compound **4**.

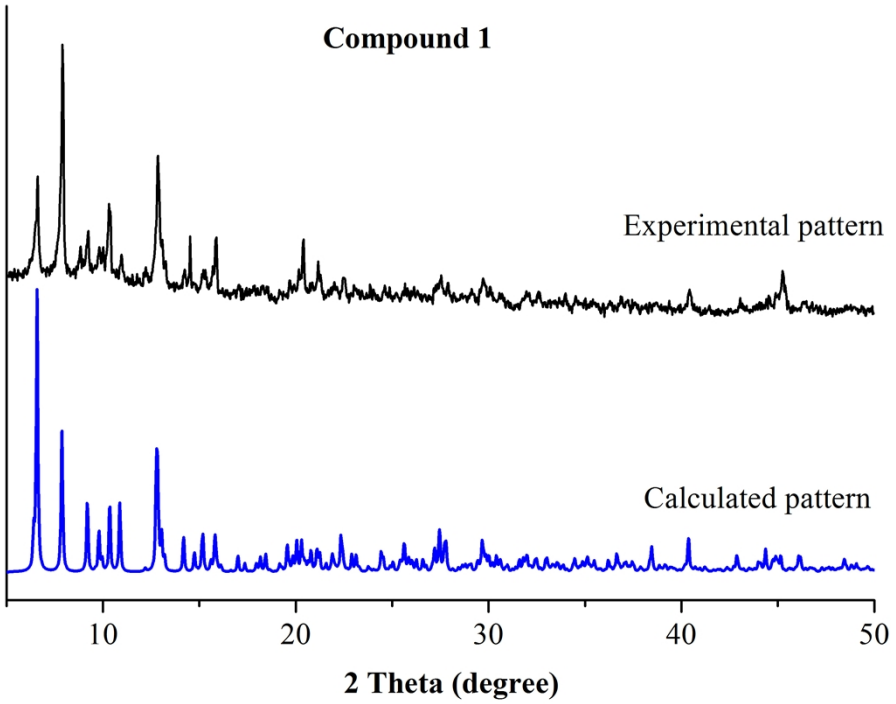

Fig. S6a The calculated and experimental PXRD patterns for compound **1**.

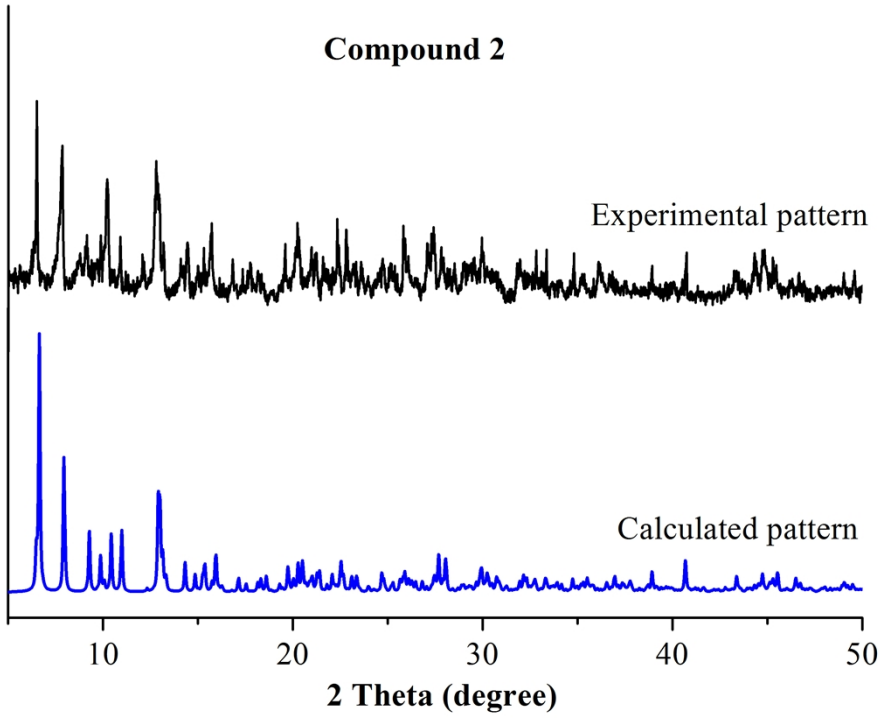

Fig. S6b The calculated and experimental PXRD patterns for compound **2**.

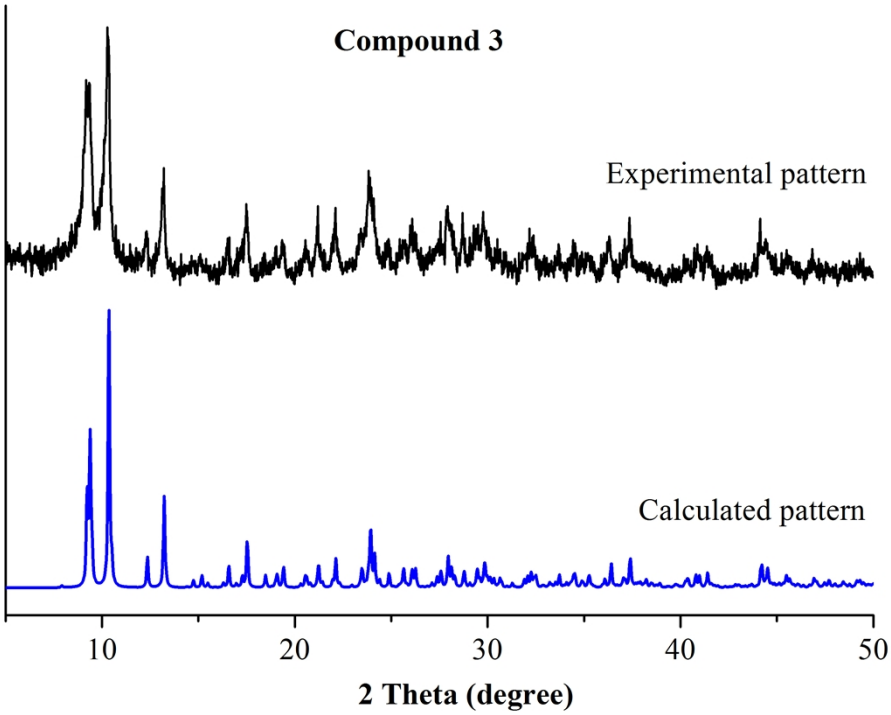

Fig. S6c The calculated and experimental PXRD patterns for compound **3**.

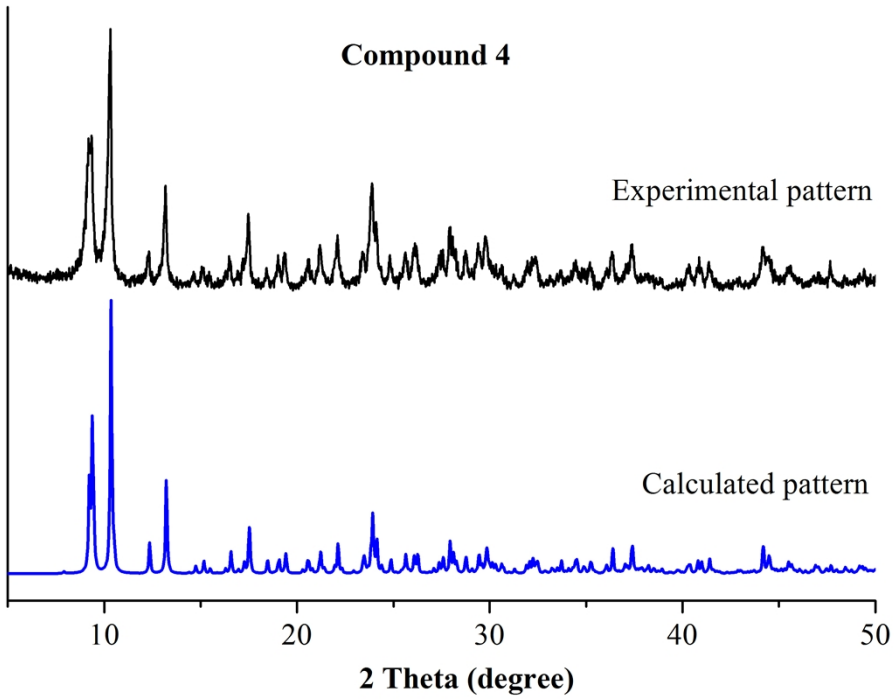

Fig. S6d The calculated and experimental PXRD patterns for compound **4**.

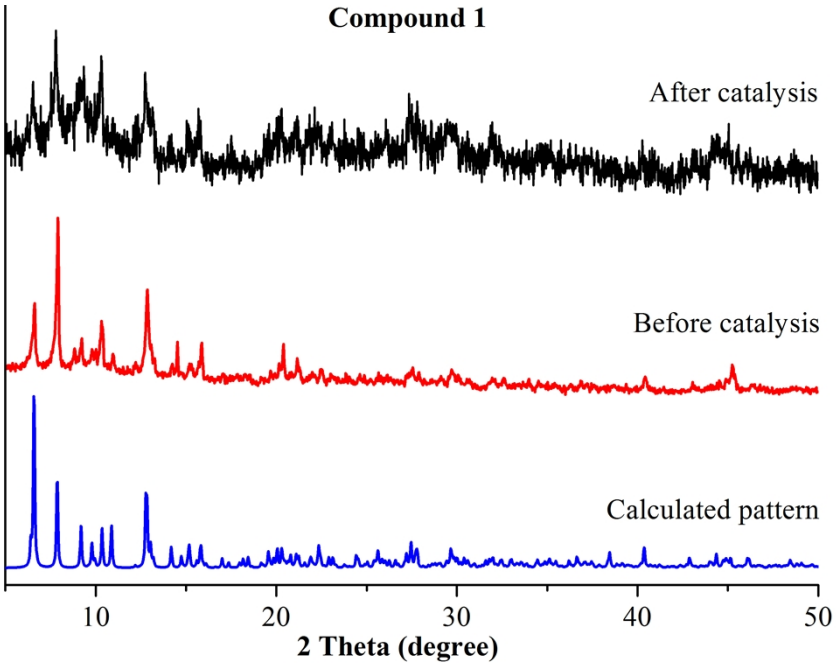

Fig. S7a Powder X-ray diffraction (PXRD) patterns of **1**: calculated pattern from crystal data (blue line); experimental pattern before catalysis (red line); recovered catalyst **1** after 3 catalytic runs of the cyanosilylation of benzaldehyde (black line).

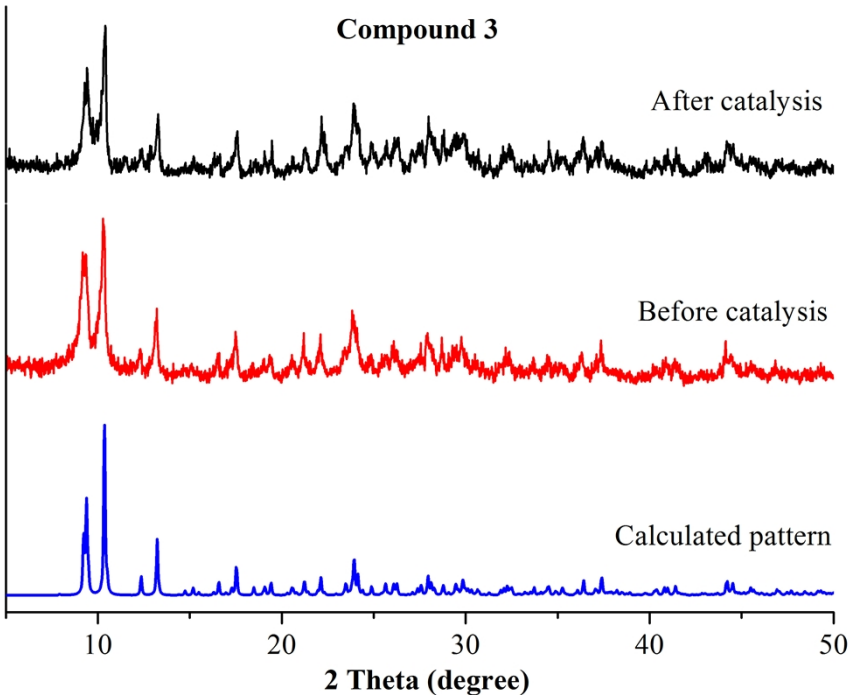

Fig. S7b Powder X-ray diffraction (PXRD) patterns of **3**: calculated pattern from crystal data (blue line); experimental pattern before catalysis (red line); recovered catalyst **3** after 3 catalytic runs of the cyanosilylation of benzaldehyde (black line).

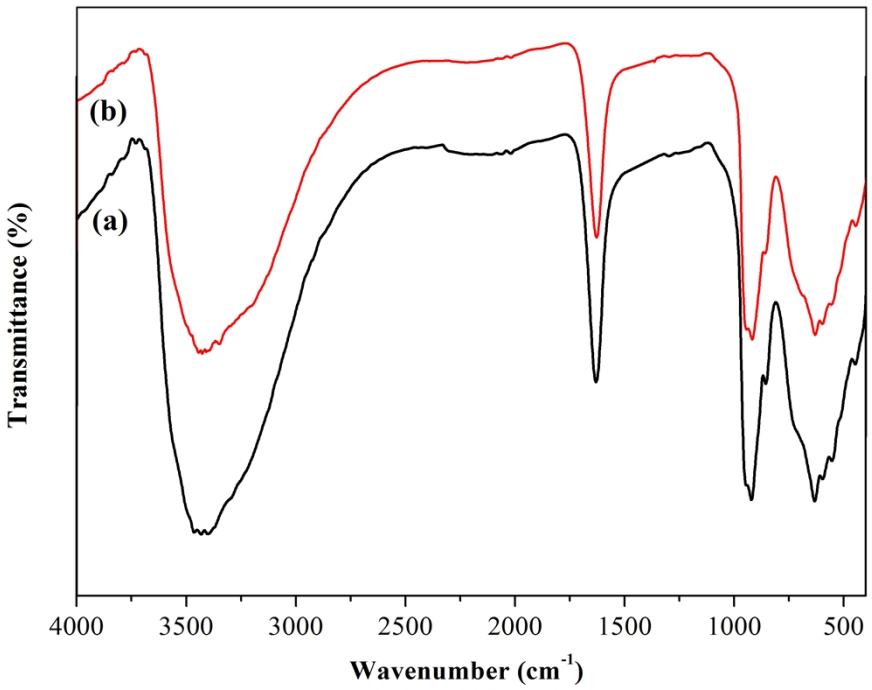

Fig. S8a IR spectrum for (a) as-synthesized compound **1** and (b) recovered catalyst after catalysis reaction.

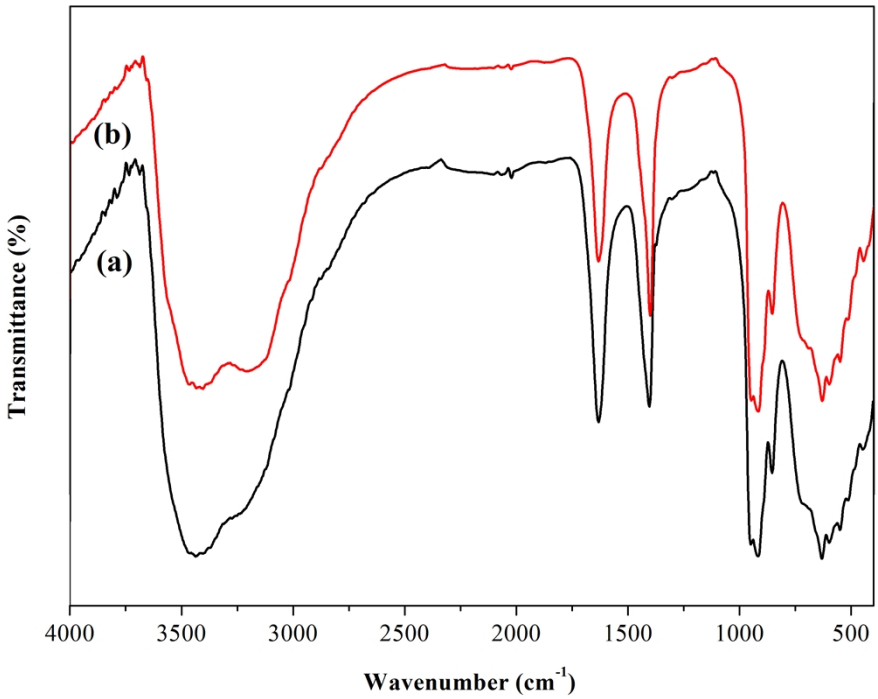

Fig. S8b IR spectrum for (a) as-synthesized compound **3** and (b) recovered catalyst after catalysis reaction.

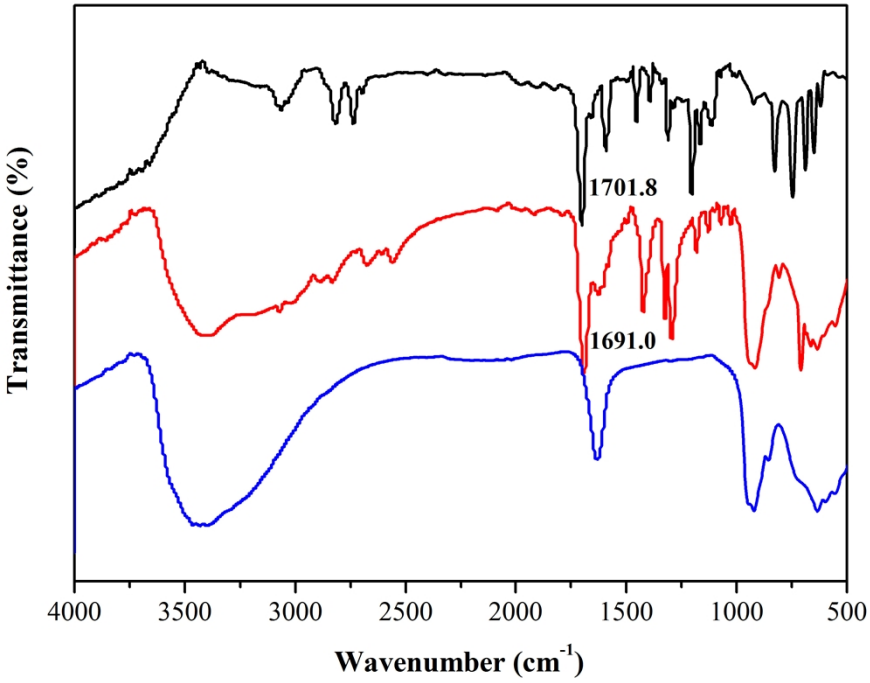

Fig. S9a IR spectra of **1** (bottom), benzaldehyde (top), and **1** obtained after the absorption of benzaldehyde (middle).

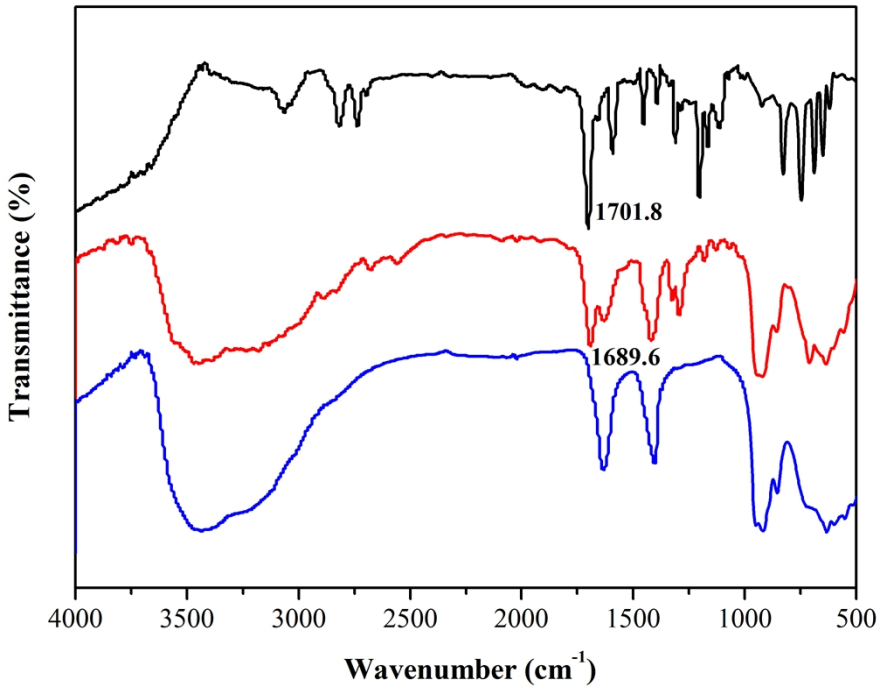

Fig. S9b IR spectra of **3** (bottom), benzaldehyde (top), and **3** obtained after the absorption of benzaldehyde (middle).

III. Supplementary Tables

Table S1 Selected bond lengths (Å) and angles (°) for **1** and **3**.

		Compound **1**[a]	
Mo(9)-O(12)	1.681(6)	Mo(4)-O(28)	1.713(6)
Mo(6)-O(14)	1.725(6)	Mo(9)-O(27)	1.728(6)
Mo(6)-O(17)	1.874(6)	Mo(9)-O(4)	2.229(5)
Mo(2)-O(9)	1.972(6)	Mo(8)-O(32)	2.288(6)
Mo(5)-O(20)	1.989(5)	Mo(1)-O(5)	2.222(5)
Mo(9)-O(3)	2.363(5)	Mo(5)-O(5)	2.333(5)
Co(1)-O(5)	1.871(5)	Co(2)-O(4)	1.958(5)
Sm(1)-O(4W)	2.399(6)	Sm(2)-O(11W)	2.430(7)
Sm(1)-O(3W)	2.405(7)	Sm(2)-O(9W)	2.450(7)
Sm(1)-O(1W)	2.437(8)	Sm(2)-O(10W)	2.457(7)
Sm(1)-O(10)	2.448(5)	Sm(2)-O(12W)	2.461(8)
Sm(1)-O(5W)	2.450(6)	Sm(2)-O(28)	2.483(6)
Sm(1)-O(27)	2.456(6)	Sm(2)-O(8W)	2.483(7)
Sm(1)-O(34)#1	2.511(6)	Sm(2)-O(6W)	2.489(8)
Sm(1)-O(2W)	2.557(8)	Sm(2)-O(38)#2	2.526(6)
Sm(1)-O(11)	2.628(6)	Sm(2)-O(7W)	2.539(8)
O(8)-Co(2)-O(5)	83.5(2)	O(5)-Co(2)-O(32)	175.8(2)
		Compound **3**	
Mo(2)-O(15)	1.682(5)	Mo(1)-O(35)	1.727(5)
Mo(5)-O(28)	1.730(5)	Mo(2)-O(31)	1.740(5)
Mo(10)-O(22)	1.847(5)	Mo(2)-O(23)	2.233(5)
Mo(2)-O(7)	1.987(5)	Mo(8)-O(21)	2.287(5)
Mo(5)-O(2)	1.980(5)	Mo(1)-O(14)	2.210(5)
Mo(7)-O(2)	2.369(5)	Mo(5)-O(12)	2.363(5)
Co(1)-O(8)	1.857(4)	Co(2)-O(38)	1.936(5)
Sm(1)-O(6W)	2.437(6)	Sm(1)-O(35)	2.483(5)
Sm(1)-O(10)	2.446(5)	Sm(1)-O(31)	2.491(5)
Sm(1)-O(1W)	2.465(5)	Sm(1)-O(2W)	2.491(6)
Sm(1)-O(4W)	2.473(6)	Sm(1)-O(5W)	2.523(6)
Sm(1)-O(3W)	2.483(7)		
O(23)-Co(1)-O(6)	83.8(2)	O(12)-Co(2)-O(38)	175.9(2)

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

Table S2 Study on recycling of catalysts **1** and **3** for the heterogeneous cyanosilylation of benzaldehyde under the similar condition.

compound	**Entry**	**Efficiency (%)**
1	Round 1	98.2
	Round 2	97.8
	Round 3	96.9
3	Round 1	98.4
	Round 2	97.1
	Round 3	96.4