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Accessory Publication

3d-4f Heterometallic Complexes for the Construction of POM-based Inorganic-Organic Hybrid Compounds: from Nanoclusters to One-Dimensional Ladder-like Chains

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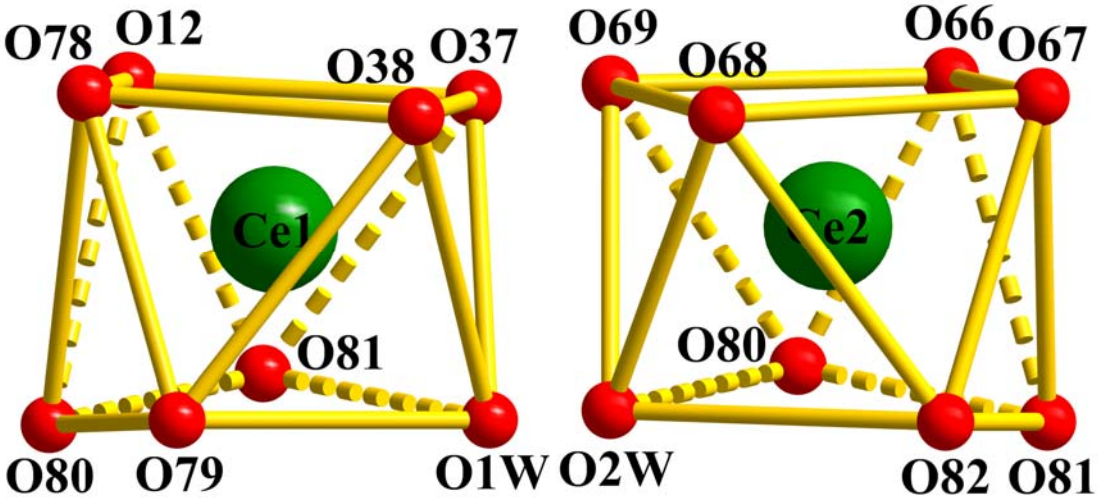


(a) (b)

Fig. S1. The square antiprismatic geometries of the Ce1 (a) and Ce2 (b) cations in compound **3**.

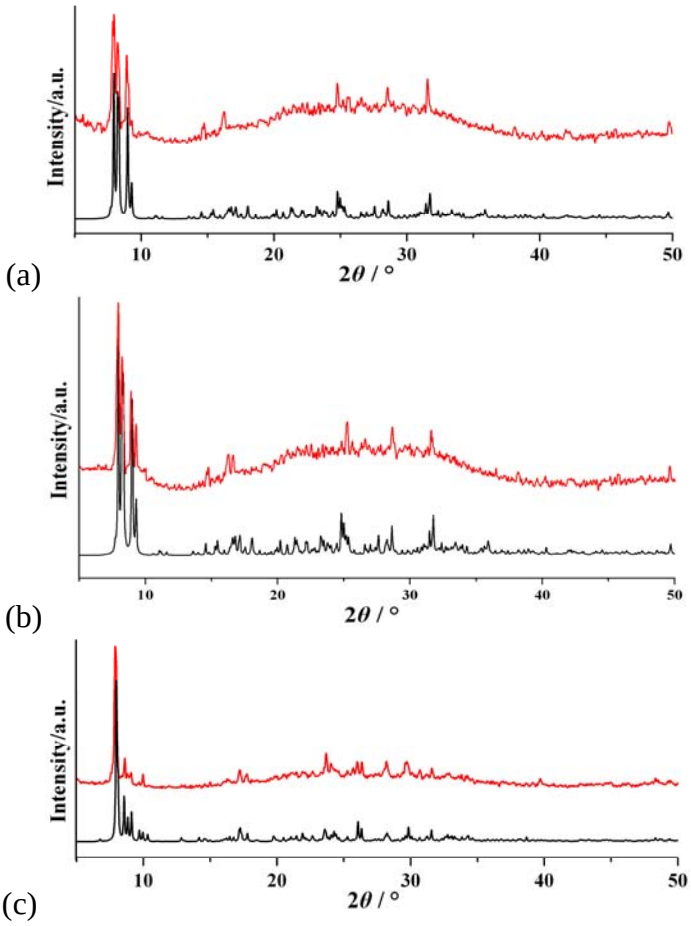
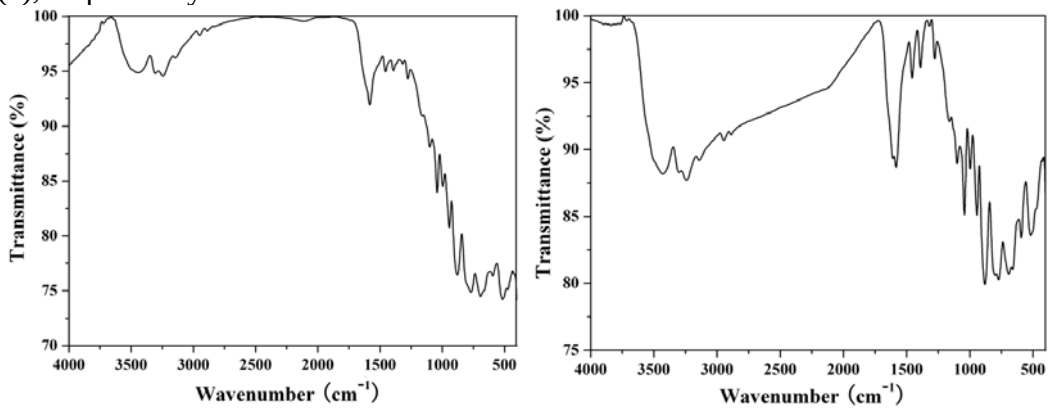
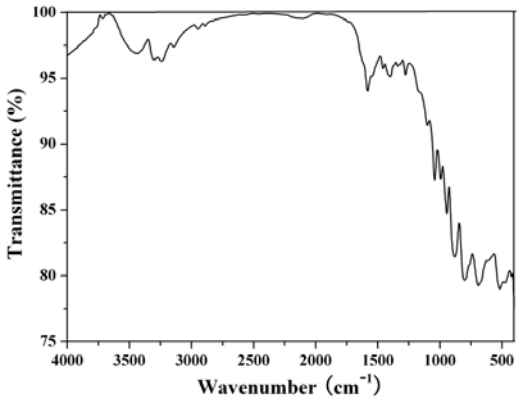


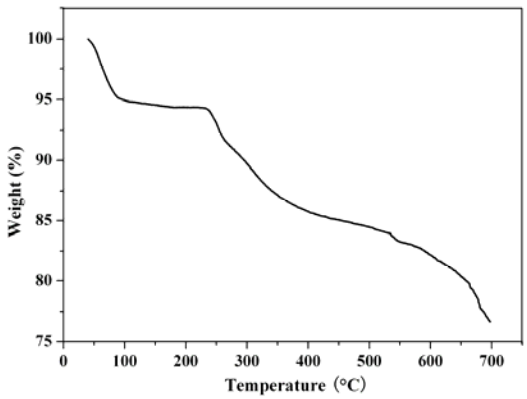
Fig. S2. The XRPD patterns (top) and simulated patterns (bottom) of **1** (a), **2** (b), and **3** (c), respectively.



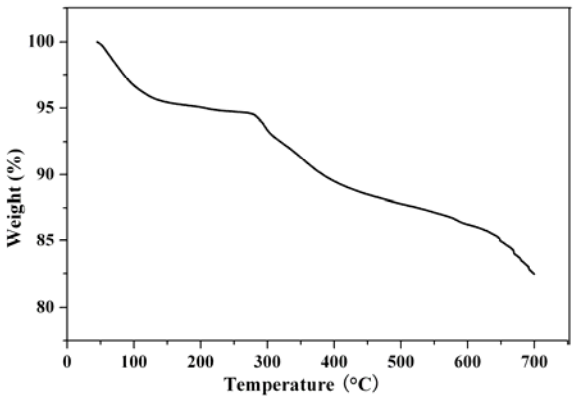


(c)

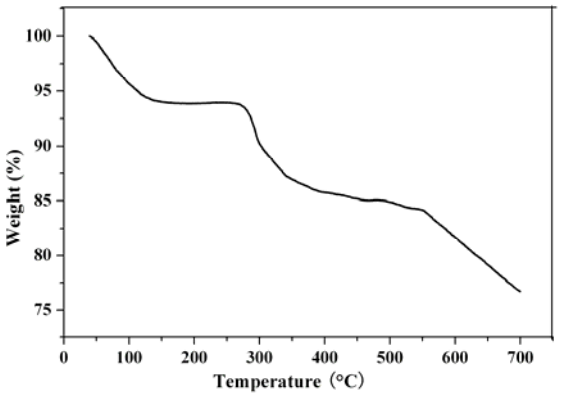
Fig. S3. The IR spectra of **1** (a), **2** (b) and **3** (c) in KBr pellets, respectively.



(a)



(b)



(c)

Fig. S4. The TGA curves of **1** (a), **2** (b) and **3** (c) in N_2 atmosphere from room temperature to 700 °C, respectively.

Table S1. Selected bond lengths [Å] and angles [deg] for **1**.

O(1W)-Nd(1)	2.550(12)	O(18)-Nd(1)-O(41)	131.1(4)
O(16)-Nd(1)	2.397(10)	O(35)-Nd(1)-O(41)	72.6(4)
O(18)-Nd(1)	2.344(10)	O(39)-Nd(1)-O(41)	81.7(4)
O(35)-Nd(1)	2.368(10)	O(16)-Nd(1)-O(41)	150.1(4)
O(39)-Nd(1)	2.371(11)	O(18)-Nd(1)-O(40)	78.6(4)
O(40)-Nd(1)	2.547(12)	O(35)-Nd(1)-O(40)	132.3(4)
O(41)-Nd(1)	2.497(10)	O(39)-Nd(1)-O(40)	144.9(4)
O(41)-Nd(1)#1	2.604(11)	O(16)-Nd(1)-O(40)	80.2(4)
		O(41)-Nd(1)-O(40)	103.6(4)
O(18)-Nd(1)-O(35)	71.2(4)	O(18)-Nd(1)-O(1W)	145.8(4)
O(18)-Nd(1)-O(39)	124.2(4)	O(35)-Nd(1)-O(1W)	142.9(4)
O(35)-Nd(1)-O(39)	82.7(4)	O(39)-Nd(1)-O(1W)	75.1(4)
O(18)-Nd(1)-O(16)	78.8(4)	O(16)-Nd(1)-O(1W)	78.0(4)
O(35)-Nd(1)-O(16)	126.7(4)	O(41)-Nd(1)-O(1W)	75.0(4)
O(39)-Nd(1)-O(16)	79.2(4)	O(40)-Nd(1)-O(1W)	73.0(4)

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

Table S2. Selected bond lengths [Å] and angles [deg] for **2**.

O(1W)-Sm(1)	2.519(14)	O(37)-Sm(1)-O(41)	132.1(6)
O(36)-Sm(1)	2.348(15)	O(36)-Sm(1)-O(41)	73.4(5)
O(37)-Sm(1)	2.352(15)	O(39)-Sm(1)-O(41)	81.8(5)
O(38)-Sm(1)	2.397(15)	O(38)-Sm(1)-O(41)	149.6(5)
O(39)-Sm(1)	2.357(14)	O(37)-Sm(1)-O(40)	77.5(5)
O(40)-Sm(1)	2.497(14)	O(36)-Sm(1)-O(40)	132.4(6)
O(41)-Sm(1)	2.465(16)	O(39)-Sm(1)-O(40)	144.4(5)
O(41)-Sm(1)#1	2.578(15)	O(38)-Sm(1)-O(40)	79.0(5)
		O(41)-Sm(1)-O(40)	103.8(5)
O(37)-Sm(1)-O(36)	71.9(6)	O(37)-Sm(1)-O(1W)	145.5(6)
O(37)-Sm(1)-O(39)	124.8(5)	O(36)-Sm(1)-O(1W)	142.5(6)
O(36)-Sm(1)-O(39)	83.1(5)	O(39)-Sm(1)-O(1W)	74.5(5)
O(37)-Sm(1)-O(38)	78.3(5)	O(38)-Sm(1)-O(1W)	78.1(5)
O(36)-Sm(1)-O(38)	127.2(5)	O(41)-Sm(1)-O(1W)	73.9(6)
O(39)-Sm(1)-O(38)	79.6(5)	O(40)-Sm(1)-O(1W)	73.5(6)

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

Table S3. Selected bond lengths [Å] and angles [deg] for **3**.

O(1W)-Ce(1)	2.57(2)	O(79)-Ce(1)-O(1W)	75.3(8)
O(12)-Ce(1)	2.395(13)	O(37)-Ce(1)-O(80)	148.6(5)
O(37)-Ce(1)	2.383(17)	O(12)-Ce(1)-O(80)	85.2(5)
O(38)-Ce(1)	2.451(13)	O(78)-Ce(1)-O(80)	80.4(5)
O(78)-Ce(1)	2.411(17)	O(38)-Ce(1)-O(80)	134.5(5)
O(79)-Ce(1)	2.566(17)	O(81)-Ce(1)-O(80)	65.7(4)
O(80)-Ce(1)	2.658(16)	O(79)-Ce(1)-O(80)	49.6(5)
O(81)-Ce(1)	2.537(14)	O(1W)-Ce(1)-O(80)	97.8(6)
O(2W)-Ce(2)	2.567(16)	O(66)-Ce(2)-O(67)	71.6(5)
O(66)-Ce(2)	2.399(13)	O(66)-Ce(2)-O(69)	80.9(5)
O(67)-Ce(2)	2.407(16)	O(67)-Ce(2)-O(69)	120.5(5)
O(68)-Ce(2)	2.441(14)	O(66)-Ce(2)-O(68)	122.8(5)
O(69)-Ce(2)	2.415(15)	O(67)-Ce(2)-O(68)	77.3(5)
O(80)-Ce(2)	2.479(13)	O(69)-Ce(2)-O(68)	75.3(5)
O(81)-Ce(2)	2.623(15)	O(66)-Ce(2)-O(80)	73.3(5)
O(82)-Ce(2)	2.550(17)	O(67)-Ce(2)-O(80)	132.4(5)
O(37)-Ce(1)-O(12)	81.0(5)	O(69)-Ce(2)-O(80)	83.8(5)
O(37)-Ce(1)-O(78)	120.5(5)	O(68)-Ce(2)-O(80)	150.0(6)
O(12)-Ce(1)-O(78)	70.6(5)	O(66)-Ce(2)-O(82)	128.5(5)
O(37)-Ce(1)-O(38)	76.2(5)	O(67)-Ce(2)-O(82)	75.5(6)
O(12)-Ce(1)-O(38)	121.9(5)	O(69)-Ce(2)-O(82)	150.6(5)
O(78)-Ce(1)-O(38)	76.6(5)	O(68)-Ce(2)-O(82)	85.8(6)
O(37)-Ce(1)-O(81)	83.3(5)	O(80)-Ce(2)-O(82)	103.6(6)
O(12)-Ce(1)-O(81)	73.4(4)	O(66)-Ce(2)-O(2W)	146.3(7)
O(78)-Ce(1)-O(81)	131.9(5)	O(67)-Ce(2)-O(2W)	142.1(7)
O(38)-Ce(1)-O(81)	151.2(5)	O(69)-Ce(2)-O(2W)	78.8(6)
O(37)-Ce(1)-O(79)	151.7(6)	O(68)-Ce(2)-O(2W)	77.1(6)
O(12)-Ce(1)-O(79)	127.3(6)	O(80)-Ce(2)-O(2W)	77.9(7)
O(78)-Ce(1)-O(79)	75.7(7)	O(82)-Ce(2)-O(2W)	75.1(7)
O(38)-Ce(1)-O(79)	86.6(5)	O(66)-Ce(2)-O(81)	85.1(5)
O(81)-Ce(1)-O(79)	103.2(6)	O(67)-Ce(2)-O(81)	78.8(5)
O(37)-Ce(1)-O(1W)	79.4(7)	O(69)-Ce(2)-O(81)	150.2(5)
O(12)-Ce(1)-O(1W)	146.5(8)	O(68)-Ce(2)-O(81)	133.9(5)
O(78)-Ce(1)-O(1W)	142.9(8)	O(80)-Ce(2)-O(81)	67.0(5)
O(38)-Ce(1)-O(1W)	79.1(7)	O(82)-Ce(2)-O(81)	50.0(5)
O(81)-Ce(1)-O(1W)	77.4(7)	O(2W)-Ce(2)-O(81)	99.7(5)