Electronic Supplementary Material (ESI) for Dalton Transactions

Syntheses, Crystal Structures and Luminescent Properties of New Lanthanide(III) Organoarsonates

Xiang-Ying Qian,[a,b] Jian-Han Zhang,[a] Tian-Hua Zhou [a] and Jiang-Gao Mao*[a]

Supporting Materials

Table S1. Hydrogen bonds for Compounds 1, 3, 5, 6 [Å and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
Compound **1**				
O(3W)-H(3WA)...O(4)#4	0.85	1.88	2.704(4)	162.8
O(3W)-H(3WB)...O(1)#7	0.85	1.97	2.793(4)	162.5
Compound **3**				
O(2W)-H(2WB)...O(3)#8	0.85	1.92	2.680(6)	147.5
O(1W)-H(1WA)...O(3)#7	0.85	1.94	2.637(5)	139.1
Compound **5**				
O(3)-H(3A)...O(7)#6	0.82	1.90	2.702(6)	164.7
O(1W)-H(1WA)...O(4)#7	0.85	1.95	2.689(7)	144.9
O(1W)-H(1WB)...O(8)#2	0.85	2.10	2.838(7)	147.8
Compound **6**				
O(3)-H(3A)...O(7)#6	0.82	1.90	2.689(1)	164.7
O(1W)-H(1WA)...O(4)#7	0.85	1.95	2.70(1)	144.9
O(1W)-H(1WB)...O(8)#2	0.85	2.10	2.847(9)	147.2

Symmetry transformations used to generate equivalent atoms:

For **1**: #4 -x-1/2, y-1/2, -z-1/2; #7 x, y, z+1.

For **3**: #7 -x+1, y+1/2, -z+1/2 ; #8 x-1, -y+1/2, z-1/2

For **5** and **6**: #2 -x+1, -y+2, -z+1; #6 x, y, z+1; #7 -x+1/2, y-1/2, -z+3/2.

Table S2. π···π packing interactions in compounds **1**, **3**, **5** and **6**.

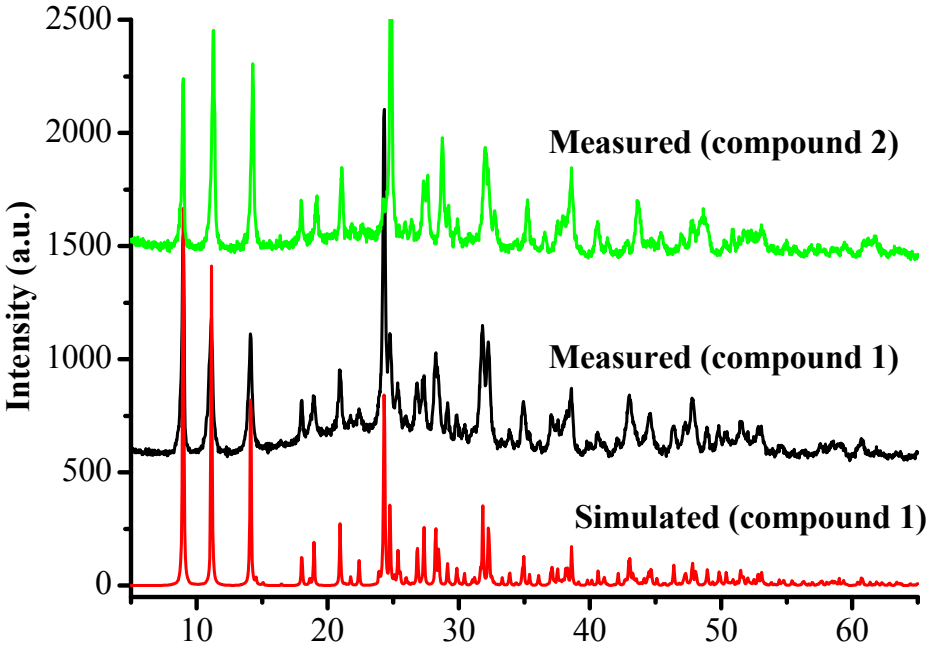
Ring System	distance (Å), dihedral angle (°)
Compound **1**	
[C(1), C(2), C(3), C(4), C(5), C(6)]…	4.230, 0
[C(1), C(2), C(3), C(4), C(5), C(6)]#1	
[C(1), C(2), C(3), C(4), C(5), C(6)]…	4.439, 0
[C(1), C(2), C(3), C(4), C(5), C(6)]#2	
Compound **3**	
[C(1), C(2), C(3), C(4), C(5), C(6)]…	3.566, 2.2
[C(1), C(2), C(3), C(4), C(5), C(6)]#1	
Compound **5**	
[C(1), C(2), C(3), C(4), C(5), C(6)]…	4.347, 2.5
[C(1), C(2), C(3), C(4), C(5), C(6)]#1	
Compound **6**	
[C(1), C(2), C(3), C(4), C(5), C(6)]…	4.330, 2.3
[C(1), C(2), C(3), C(4), C(5), C(6)]#1	

Symmetry transformations used to generate equivalent atoms:

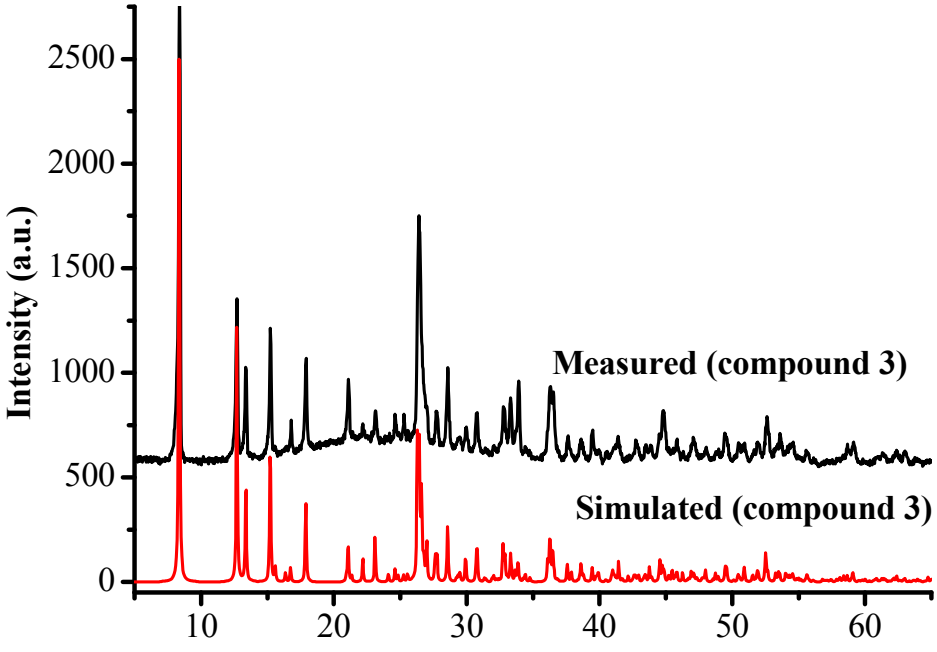
For **1**: #1 1-x, 1-y, -z; #2 –x, 1-y, -1-z

For **3**: #1 x, 1/2-y, -1/2+z

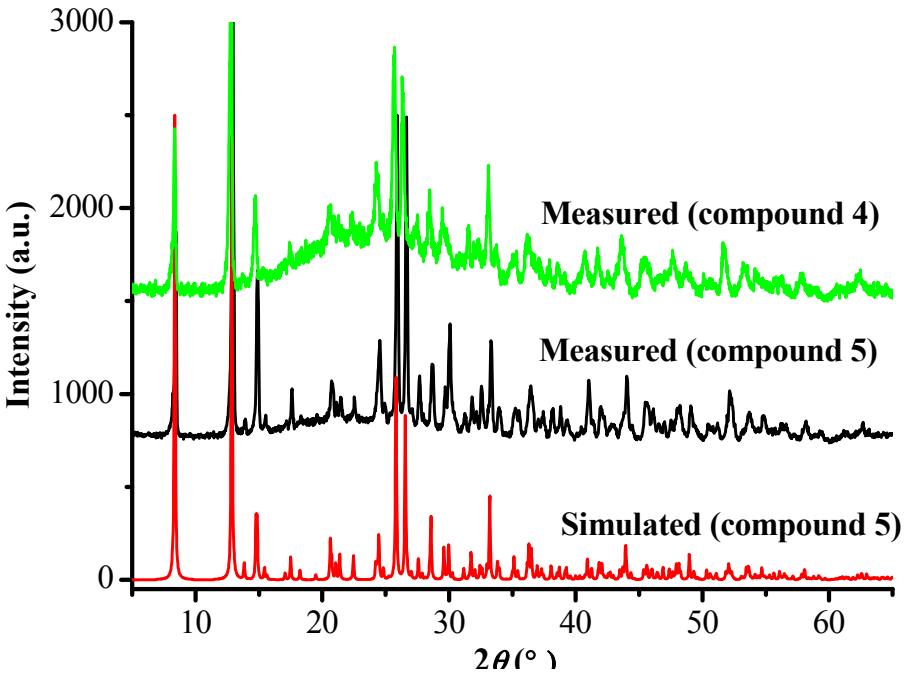
For **5** and **6** : #1 -1/2+x, 5/2-y, -1/2+z



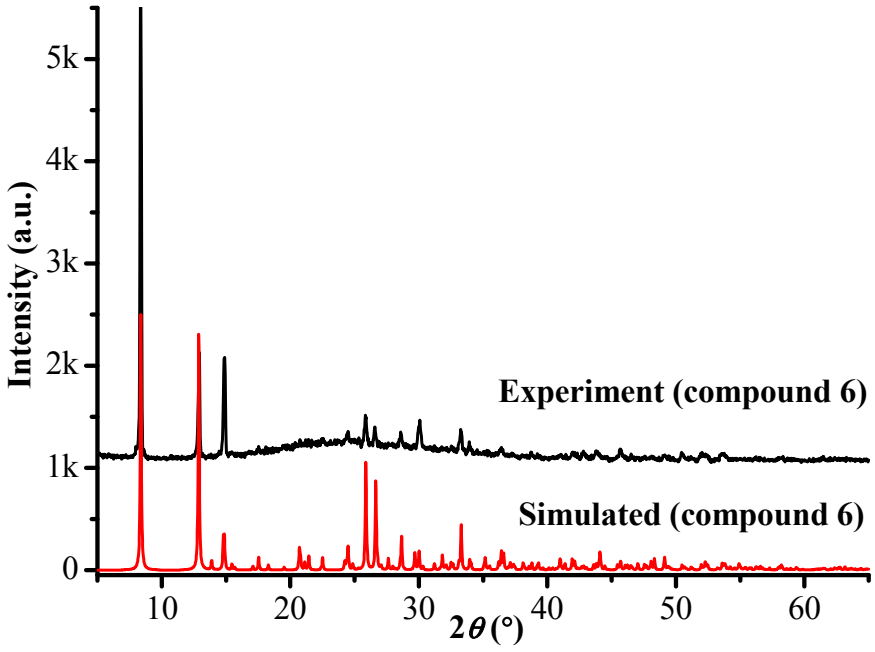
(a)



(b)



(c)



(d)

Figure S1. Simulated and measured XRD powder patterns for compounds **1-6**.

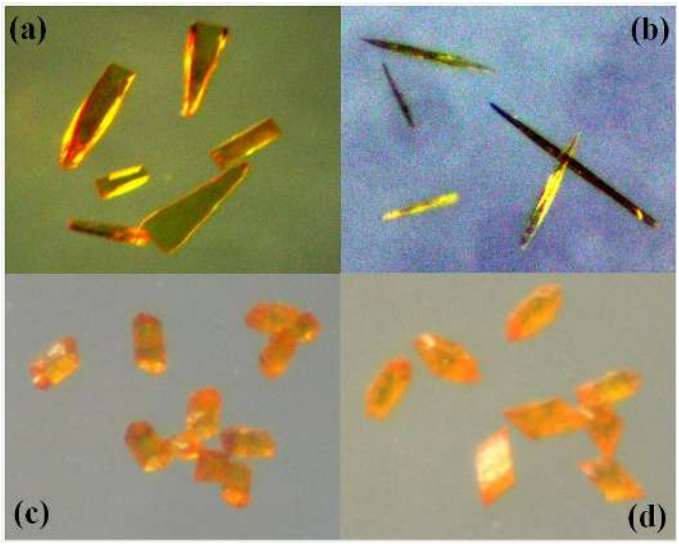


Figure S2. Morphologies of compounds **1** (a), **3** (b), **5** (c) and **6** (d).

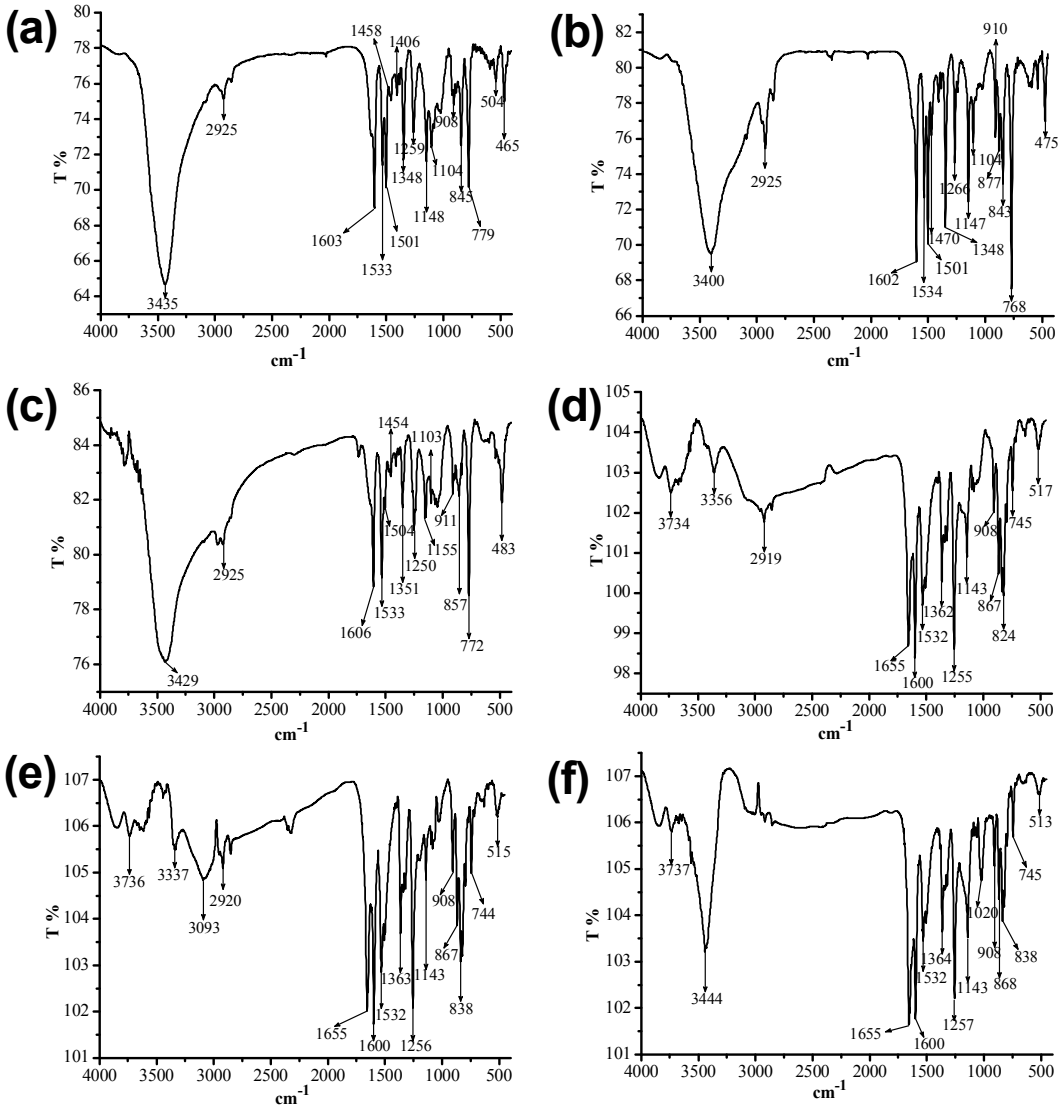
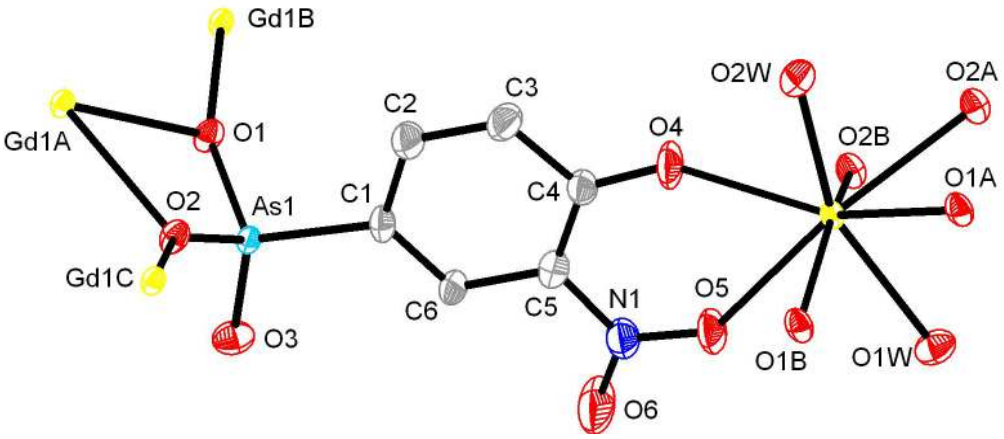
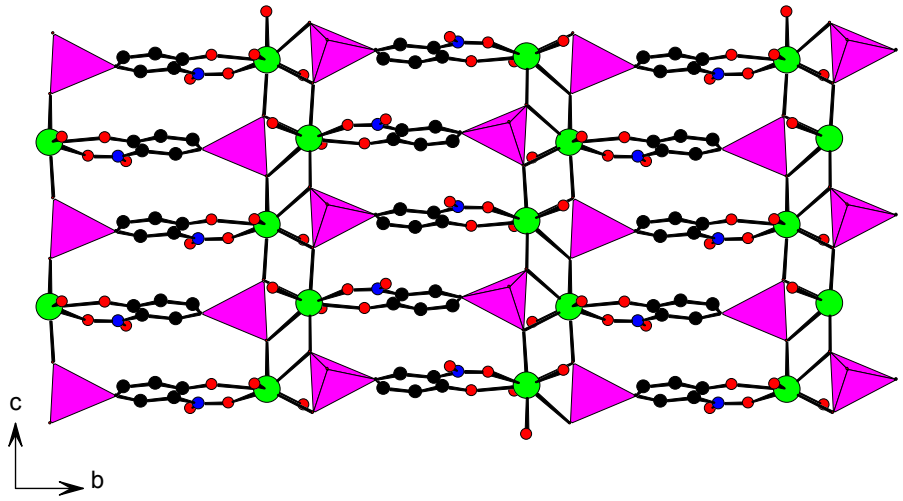


Figure S3. IR spectra of compounds **1** (a), **2** (b), **3** (c), **4** (d), **5** (e) and **6** (f).



(a)



(b)

Figure S4. ORTEP representation of the selected unit in compound **3**. The thermal ellipsoids are drawn at 50% probability level (a), a 2D layer perpendicular to the *a*-axis (b). C-AsO_3 groups are shaded as pick tetrahedral, Gd, O, N and C atoms are drawn as green, red, blue and black circles, respectively.