Supporting information

Lanthanide Diphosphonates Based on V-shaped Rigid Ligand: Syntheses, Structures, Experimental and Theoretical Luminescence Properties.
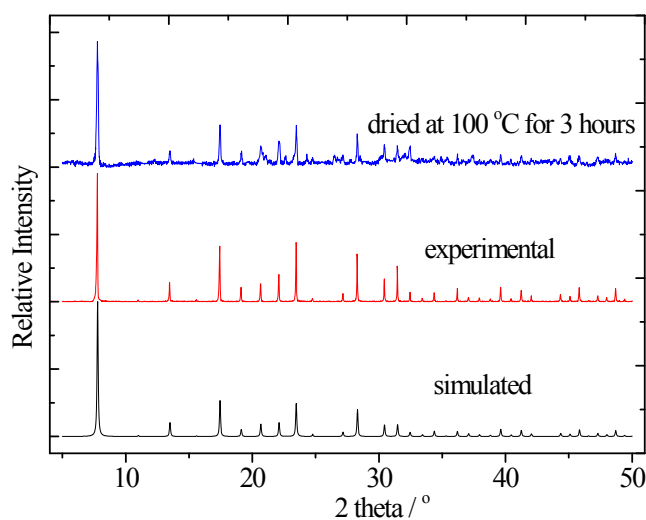
Si-Fu Tang and Xuebing Li

Figure S1. Comparison of simulated and experimental PXRD diagrams of compound **1**.
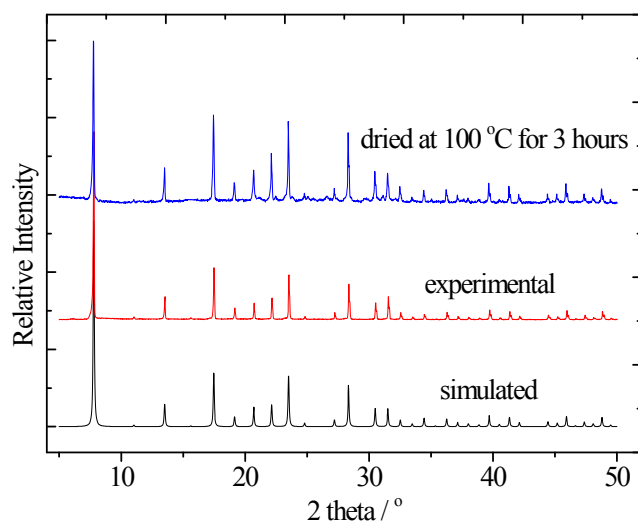

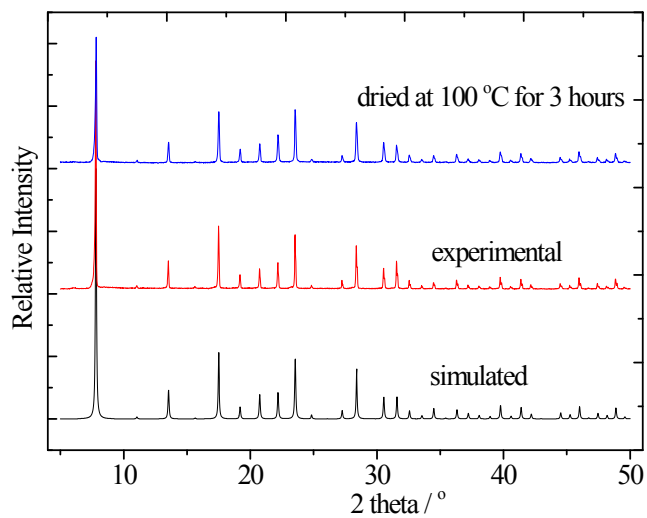Figure S2. Comparison of simulated and experimental PXRD diagrams of compound

2.

dried at 100 °C for 3 hours

experimental

simulated

Relative Intensity

2 theta / °

Figure S3. Comparison of simulated and experimental PXRD diagrams of compound

3.

dried at 100 °C for 3 hours

experimental

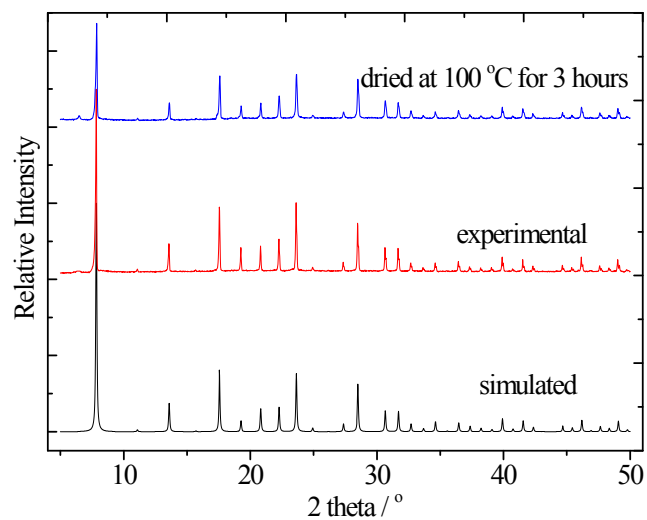simulated

Relative Intensity

2 theta / °

Figure S4. Comparison of simulated and experimental PXRD diagrams of compound

4.
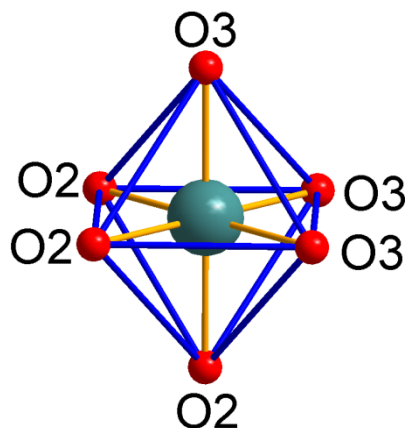
Figure S5. Coordination environment in compounds **1-4**.

Table S1. Selected angles found in compounds **1-4**.

Compound **1**		Compound **2**	
O(2)-Eu(1)-O(2)#1	89.90(7)	O(2)-Gd(1)-O(2)#1	90.52(6)
O(2)-Eu(1)-O(2)#2	89.90(7)	O(2)-Gd(1)-O(2)#2	90.52(6)
O(2)#1-Eu(1)-O(2)#2	89.90(7)	O(2)#1-Gd(1)-O(2)#2	90.52(6)
O(2)-Eu(1)-O(3)#3	89.80(7)	O(2)-Gd(1)-O(3)#3	89.10(6)
O(2)#1-Eu(1)-O(3)#3	179.70(7)	O(2)#1-Gd(1)-O(3)#3	179.21(6)
O(2)#2-Eu(1)-O(3)#3	90.12(7)	O(2)#2-Gd(1)-O(3)#3	90.18(6)
O(2)-Eu(1)-O(3)#4	179.70(7)	O(2)-Gd(1)-O(3)#4	179.20(6)
O(2)#1-Eu(1)-O(3)#4	90.12(7)	O(2)#1-Gd(1)-O(3)#4	90.18(6)
O(2)#2-Eu(1)-O(3)#4	89.80(7)	O(2)#2-Gd(1)-O(3)#4	89.10(6)
O(3)#3-Eu(1)-O(3)#4	90.17(7)	O(3)#3-Gd(1)-O(3)#4	90.20(6)
O(2)-Eu(1)-O(3)#5	90.12(7)	O(2)-Gd(1)-O(3)#5	90.18(6)
O(2)#1-Eu(1)-O(3)#5	89.80(7)	O(2)#1-Gd(1)-O(3)#5	89.10(6)
O(2)#2-Eu(1)-O(3)#5	179.70(7)	O(2)#2-Gd(1)-O(3)#5	179.21(6)
O(3)#3-Eu(1)-O(3)#5	90.17(7)	O(3)#3-Gd(1)-O(3)#5	90.20(6)
O(3)#4-Eu(1)-O(3)#5	90.17(7)	O(3)#4-Gd(1)-O(3)#5	90.20(6)
Compound **3**		Compound **4**	
O(2)#1-Tb(1)-O(2)#2	90.60(9)	O(2)-Dy(1)-O(2)#1	90.78(5)
O(2)#1-Tb(1)-O(2)	90.60(9)	O(2)-Dy(1)-O(2)#2	90.78(5)
O(2)#2-Tb(1)-O(2)	90.60(9)	O(2)#1-Dy(1)-O(2)#2	90.78(5)
O(2)#1-Tb(1)-O(3)#3	178.76(9)	O(2)-Dy(1)-O(3)#3	88.70(5)
O(2)#2-Tb(1)-O(3)#3	88.81(9)	O(2)#1-Dy(1)-O(3)#3	178.86(5)
O(2)-Tb(1)-O(3)#3	90.49(10)	O(2)#2-Dy(1)-O(3)#3	90.24(5)
O(2)#1-Tb(1)-O(3)#4	90.50(10)	O(2)-Dy(1)-O(3)#4	178.86(5)
O(2)#2-Tb(1)-O(3)#4	178.76(9)	O(2)#1-Dy(1)-O(3)#4	90.24(5)
O(2)-Tb(1)-O(3)#4	88.81(9)	O(2)#2-Dy(1)-O(3)#4	88.70(5)
O(3)#3-Tb(1)-O(3)#4	90.10(9)	O(3)#3-Dy(1)-O(3)#4	90.29(5)

O(2)#1-Tb(1)-O(3)#5	88.81(9)	O(2)-Dy(1)-O(3)#5	90.25(5)
O(2)#2-Tb(1)-O(3)#5	90.50(10)	O(2)#1-Dy(1)-O(3)#5	88.70(5)
O(2)-Tb(1)-O(3)#5	178.76(10)	O(2)#2-Dy(1)-O(3)#5	178.86(5)
O(3)#3-Tb(1)-O(3)#5	90.10(9)	O(3)#3-Dy(1)-O(3)#5	90.29(5)
O(3)#4-Tb(1)-O(3)#5	90.10(9)	O(3)#4-Dy(1)-O(3)#5	90.29(5)

Symmetry transformations used to generate equivalent atoms: For **1**: #1 z+1, x, y-1; #2 y, z+1, x-1; #3 x+0,-y+2,-z+1/2; #4 -y+2, -z+3/2, x-1; #5 -z+3/2, x+0, -y+1; #6 -x+5/2, y+0, -z+0. For **2**: #1 z+1, x, y-1; #2 y, z+1, x-1; #3 x+0, -y+2, -z+1/2; #4 -y+2, -z+3/2, x-1; #5 -z+3/2, x+0, -y+1; #6 -x+5/2, y+0, -z+0. For **3**: #1 y, z-1, x+1; #2 z-1, x, y+1; #3 x+0, -y+0, -z+3/2; #4 -z+1/2, x+0, -y+1; #5 -y+0, -z+1/2, x+1; #6 -x-1/2, y+0, -z+2. For **4**: #1 z+1, x, y-1; #2 y, z+1, x-1; #3 -z+3/2, x+0, -y+1; #4 -y+2, -z+3/2, x-1; #5 x+0, -y+2, -z+1/2; #6 -x+5/2, y+0, -z+0.
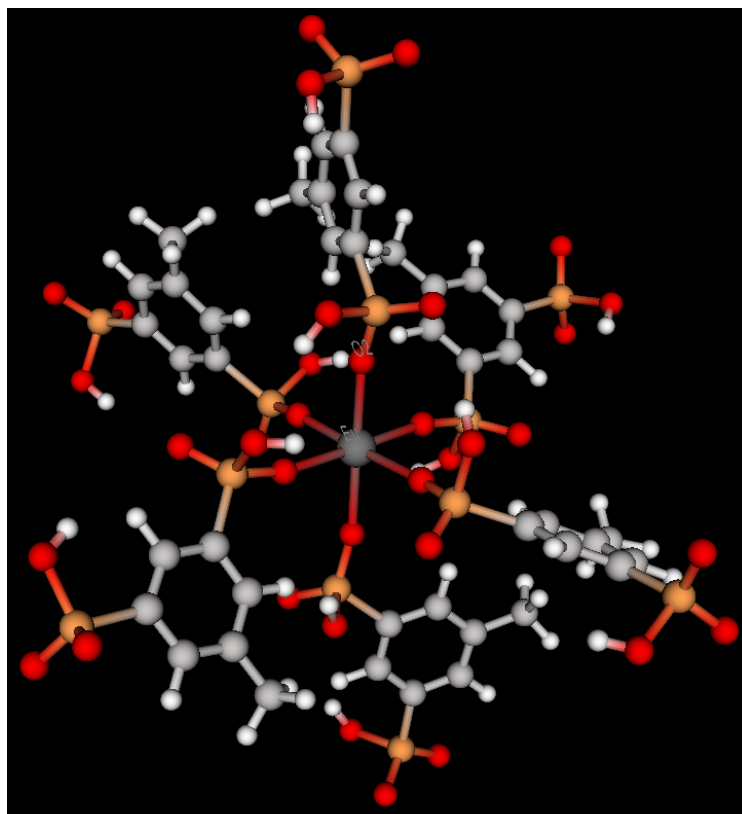

Figure S6. Optimized geometry using sparkle PM3 implemented in the MOPAC 2012