Supporting Information

High-energy-density materials with remarkable thermostability and insensitivity: synthesis, structures and physicochemical properties of Pb(II) compounds based on 3-(tetrazol-5-yl)triazole as ligand

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

Pb(1)-N(14)	2.707(7)	Pb(1)-N(1)	2.724(6)
Pb(1)-N(5)#1	2.721(7)	Pb(1)-N(11)#2	2.738(6)
Pb(1)-O(1)	2.722(6)	Pb(1)-N(8)	2.800(7)
Pb(1)-N(4)#1	2.821(6)	N(4)#1-Pb(1)-N(14)	131.992
N(14)-Pb(1)-N(5)#1	88.6(2)	C(1)-N(1)-Pb(1)	119.7(5)
N(14)-Pb(1)-O(1)	69.50(19)	N(2)-N(1)-Pb(1)	136.0(5)
N(5)#1-Pb(1)-O(1)	72.49(18)	C(6)-N(13)-H(13)	127(6)
N(14)-Pb(1)-N(1)	142.6(2)	C(3)-N(5)-Pb(1)#3	139.8(5)
N(5)#1-Pb(1)-N(1)	88.0(2)	C(2)-N(5)-Pb(1)#3	117.1(5)
O(1)-Pb(1)-N(1)	73.93(18)	C(6)-N(14)-Pb(1)	139.6(6)
N(14)-Pb(1)-N(11)#2	80.1(2)	C(5)-N(14)-Pb(1)	117.4(5)
N(5)#1-Pb(1)-N(11)#2	140.8(2)	C(4)-N(8)-Pb(1)	114.9(5)
O(1)-Pb(1)-N(11)#2	68.34(17)	N(9)-N(8)-Pb(1)	141.1(5)
N(1)-Pb(1)-N(11)#2	79.3(2)	C(4)-N(11)-Pb(1)#4	116.2(5)
N(5)#1-Pb(1)-N(8)	79.5(2)	N(10)-N(11)-Pb(1)#4	138.8(5)
O(1)-Pb(1)-N(8)	124.68(18)	Pb(1)-O(1)-H(1A)	125.4
N(1)-Pb(1)-N(8)	151.7(2)	Pb(1)-O(1)-H(1B)	109.3
N(11)#2-Pb(1)-N(8)	125.6(2)	N(4)#1-Pb(1)-N(5)#1	62.990
N(4)#1-Pb(1)-N(11)#2	145.962	N(4)#1-Pb(1)-N(8)	73.776
N(4)#1-Pb(1)-N(1)	77.973		

Symmetry transformations used to generate equivalent atoms:

#1 -y+1/4,x+1/4,-z+1/4; #2 -y+5/4,x+1/4,-z+1/4;

#3 y-1/4,-x+1/4,-z+1/4; #4 y-1/4,-x+5/4,-z+1/4.

Table S2. Selected bond lengths (Å) and bond angles (°) for **2.**

Pb(1)-O(1)	2.363(17)	Pb(1)-N(1)	2.72(2)
Pb(1)-O(1)#1	2.466(17)	O(1)-Pb(1)#3	2.466(17)
Pb(1)-O(1)#2	2.502(13)	O(1)-Pb(1)#2	2.502(13)
O(1)-Pb(1)-O(1)#1	107.8(6)	C(2)-N(1)-Pb(1)	119.4(16)
O(1)-Pb(1)-O(1)#2	72.6(6)	C(1)-N(1)-Pb(1)	137.3(18)
O(1)#1-Pb(1)-O(1)#2	72.6(6)	Pb(1)-O(1)-Pb(1)#3	107.8(6)
O(1)-Pb(1)-N(1)	77.9(6)	Pb(1)-O(1)-Pb(1)#2	107.4(6)
O(1)#1-Pb(1)-N(1)	83.3(6)	Pb(1)#3-O(1)-Pb(1)#2	107.4(6)
O(1)#2-Pb(1)-N(1)	133.4(6)		

Symmetry transformations used to generate equivalent atoms:

#1 x+1,y,z; #2 -x+1,-y+1,-z+2; #3 x-1,y,z.

Table S3. Hydrogen-bonding interactions in **1** and **2**.

	d(D-H···A) [Å]	**d(D-H)** [Å]	**d(H…A)** [Å]	**d(D…A)** [Å]	**<(DHA)** [°]
1	O(1)-H(1A)...N(6)	0.850	2.557	3.144	127.15
	O(1)-H(1B)...N(3)	0.850	2.355	3.000	133.01
	O(1)-H(1B)...N(14)	0.850	2.697	3.095	110.23
	N(6)-H(6)...N(2)	0.888	2.122	2.896	145.23
	Symmetry transformations used to generate equivalent atoms:				
	#1 y-1/4, -x+3/4, z-1/4; #2 x, y+1/2, -z; #3 -y+3/4, x+1/4, z+1/4; #4 -y+5/4, x+3/4, z-1/4.				
2	N(2)-H(2A)...N(7)	0.860	2.002	2.851	169.18
	N(6)-H(6A)...O(1)	0.860	2.333	2.964	130.42
	Symmetry transformations used to generate equivalent atoms:				
	#1 x+1, -y+1/2, z+1/2; #2 x-1, y, z-1.				

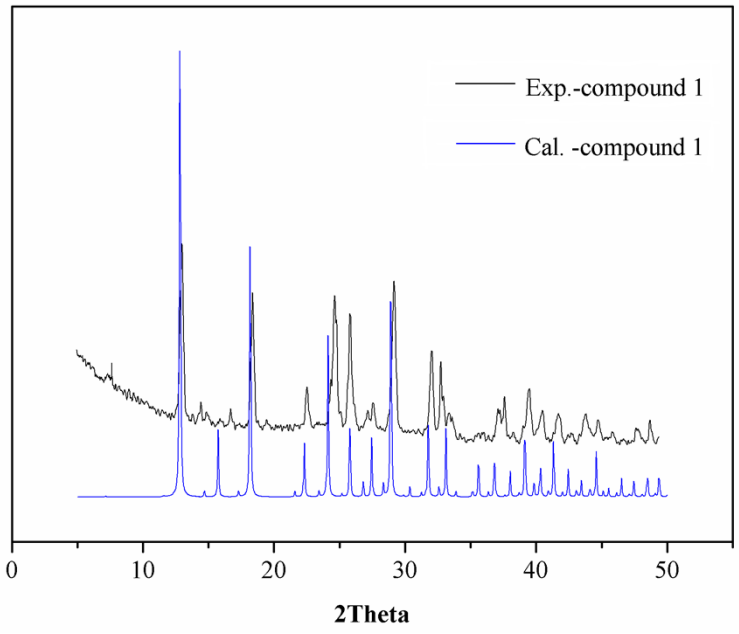

Fig. S1 XRPD curves for compound **1**.

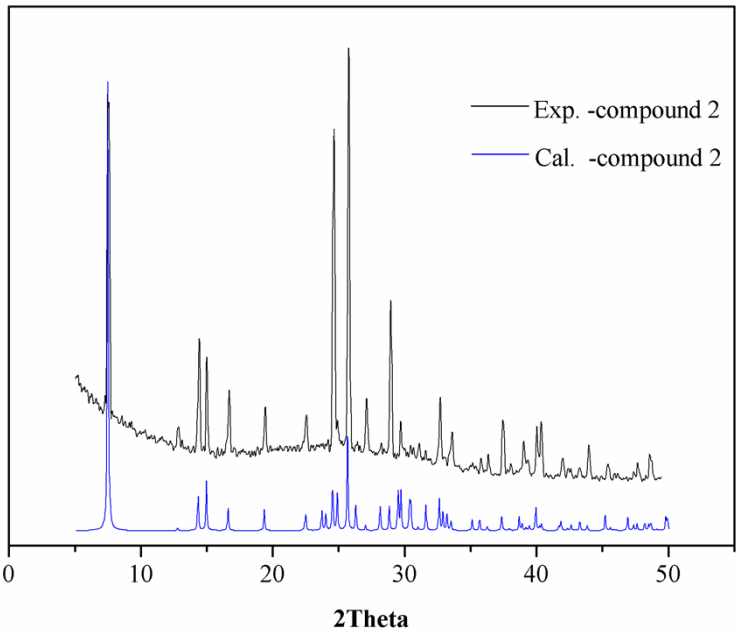

Fig. S2 XRPD curves for compound **2**.