

Lanthanide Complexes with 3, 4, 5-Triethoxybenzoic acid and 1,10-phenanthroline: Synthesis, Crystal structures, Thermal decomposition mechanism and Phase transformation kinetics

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Table S1a Experimental molar heat capacities of complexes 1-2.

Complex 1		Complex 2		Complex 1		Complex 2	
T/K	$C_{p,m}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_{p,m}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	T/K	$C_{p,m}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_{p,m}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_{p,m}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	$C_{p,m}/\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$
	1	1					
263.15	1721.939	2310.871	364.65	2559.696	3326.121		
266.65	1756.439	2350.456	368.15	2587.862	3360.933		
270.15	1790.884	2389.705	371.65	2619.712	3398.620		
273.65	1825.718	2428.176	375.15	2650.570	3440.145		
277.15	1859.765	2470.111	378.65	2688.824	3471.887		
280.65	1894.625	2510.252	382.15	2728.319	3486.307		
284.15	1929.270	2551.031	385.65	2769.762	3499.565		
287.65	1961.321	2592.264	389.15	2798.812	3529.956		
291.15	1993.155	2632.243	392.65	2805.194	3564.335		
294.65	2024.072	2670.498	396.15	2812.380	3600.693		
298.15	2053.150	2709.855	399.65	2823.110	3634.613		
301.65	2083.447	2745.635	403.15	2838.162	3672.571		
305.15	2115.573	2785.203	406.65	2859.083	3702.800		
308.65	2150.763	2851.476	410.15	2882.285	3736.655		
312.15	2187.285	3113.141	413.65	2907.096	3771.418		
315.65	2231.614	3554.137	417.15	2931.437	3806.982		
319.15	2287.401	3333.120	420.65	2957.197	3844.291		
322.65	2525.746	3042.193	424.15	2982.978	3880.097		
326.15	4379.366	2986.146	427.65	3012.164	3919.314		
329.65	2802.778	3011.365	431.15	3041.420	3952.391		
333.15	2385.839	3049.490	434.65	3071.835	3990.100		
336.65	2365.727	3083.507	438.15	3100.357	4028.841		
340.15	2376.015	3109.072	441.65	3129.689	4062.929		
343.65	2395.911	3137.430	445.15	3163.703	4102.665		
347.15	2419.497	3164.054	448.65	3195.861	4136.731		
350.65	2446.373	3188.143	452.15	3229.529	4174.251		
354.15	2475.413	3212.227	455.65	3264.023	4217.548		
357.65	2503.439	3245.887	459.15	3299.327	4255.997		
361.15	2530.267	3284.256	462.65	3337.430	4292.042		

Table S1b Experimental molar heat capacities of complex 3.

Complex 3		Complex 3		Complex 3	
T/K	$C_{p,m}/ \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	T/K	$C_{p,m}/ \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$	T/K	$C_{p,m}/ \text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$
263.15	2066.676	333.15	2621.097	403.15	3053.470
266.65	2093.440	336.65	2644.569	406.65	3076.679
270.15	2124.594	340.15	2662.673	410.15	3098.305
273.65	2152.957	343.65	2680.085	413.65	3120.303
277.15	2185.514	347.15	2695.012	417.15	3141.700
280.65	2215.019	350.65	2720.078	420.65	3162.120
284.15	2247.729	354.15	2749.501	424.15	3183.806
287.65	2284.440	357.65	2770.827	427.65	3207.944
291.15	2326.923	361.15	2787.315	431.15	3228.385
294.65	2387.527	364.65	2806.162	434.65	3251.338
298.15	2456.517	368.15	2828.619	438.15	3276.781
301.65	2459.154	371.65	2850.250	441.65	3298.140
305.15	2435.289	375.15	2876.534	445.15	3324.292
308.65	2441.044	378.65	2897.636	448.65	3345.645
312.15	2468.179	382.15	2918.465	452.15	3369.144
315.65	2496.898	385.65	2939.447	455.65	3388.805
319.15	2522.613	389.15	2960.555	459.15	3412.741
322.65	2546.888	392.65	2983.519	462.65	3430.878
326.15	2572.483	396.15	3004.741		
329.65	2599.667	399.65	3026.875		

Table S2a Smoothed molar heat capacities and thermodynamic functions of complex 1.

T/K	$C_{p,m}/\text{JK}^{-1}\text{mol}^{-1}$	$H_T-H_{298.15\text{K}}/\text{kJmol}^{-1}$	$S_T-S_{298.15\text{K}}/\text{JKmol}^{-1}$	$G_T-G_{298.15\text{K}}/\text{kJmol}^{-1}$
263.15	1722.14	-66.247	-235.92	-4.165
273.15	1820.65	-48.538	-169.88	-2.135
283.15	1919.41	-29.837	-102.65	-0.772
293.15	2010.37	-10.179	-34.43	-0.086
303.15	2097.02	10.395	34.57	-0.086
313.15	2199.80	31.856	104.22	-0.779
318.15	2285.09	2241138.978	7454805.36	-130607.346
328.15	3689.29	2241169.936	7454900.95	-205155.811
338.15	2267.57	2241195.158	7454976.71	-279705.218
338.65	2370.02	425.018	1381.70	-42.895
348.65	2433.71	448.996	1451.47	-57.061
358.65	2507.22	473.700	1521.33	-71.925
368.65	2594.85	499.192	1591.43	-87.488
378.65	2695.08	525.643	1662.22	-103.755
388.65	2777.91	553.034	1733.61	-120.733
398.65	2830.41	581.097	1804.90	-138.426
408.65	2873.27	609.610	1875.54	-156.828
418.65	2935.57	638.631	1945.69	-175.934
428.65	3021.44	668.404	2015.97	-195.742
438.65	3109.06	699.065	2086.67	-216.254
448.65	3191.61	730.563	2157.67	-237.476
458.65	3298.59	762.987	2229.14	-259.409

Table S2b Smoothed molar heat capacities and thermodynamic functions of complex 2.

T/K	$C_{p,m}/\text{JK}^{-1}\text{mol}^{-1}$	$H_T-H_{298.15\text{K}}/\text{kJmol}^{-1}$	$S_T-S_{298.15\text{K}}/\text{JKmol}^{-1}$	$G_T-G_{298.15\text{K}}/\text{kJmol}^{-1}$
263.15	2309.55	-87.897	-313.07	-5.511
273.15	2422.86	-64.229	-224.81	-2.822
283.15	2540.15	-39.416	-135.61	-1.019
293.15	2654.68	-13.439	-45.45	-0.114
303.15	2760.86	13.704	45.58	-0.114
306.65	2811.80	774.902	2586.72	-18.317
316.65	3572.36	806.216	2687.13	-44.662
326.65	2972.05	50.655	159.59	-1.477
336.65	3082.07	81.017	251.14	-3.530
346.65	3153.89	112.189	342.38	-6.498
356.65	3244.94	144.167	433.32	-10.376
366.65	3345.69	177.121	524.44	-15.164
376.65	3439.27	211.056	615.74	-20.864
386.65	3522.86	245.872	706.97	-27.477
396.65	3605.81	281.512	797.97	-35.002
406.65	3698.28	318.022	888.87	-43.435
416.65	3801.88	355.517	979.95	-52.779
426.65	3909.08	394.073	1071.39	-63.035
436.65	4012.23	433.684	1163.15	-74.207
446.65	4114.85	474.316	1255.15	-86.298
456.65	4228.24	516.022	1347.49	-99.310

Table S2c Smoothed molar heat capacities and thermodynamic functions of complex 3.

T/K	$C_{p,m}/\text{JK}^{-1}\text{mol}^{-1}$	$H_T-H_{298.15\text{K}}/\text{kJmol}^{-1}$	$S_T-S_{298.15\text{K}}/\text{JKmol}^{-1}$	$G_T-G_{298.15\text{K}}/\text{kJmol}^{-1}$
263.15	2066.69	6679.823	22557.33	743.860
273.15	2148.53	6700.895	22635.92	517.894
280.15	2209.54	-41.668	-144.07	-1.306
290.15	2311.12	-19.074	-64.84	-0.261
300.15	2468.13	4.954	16.56	-0.017
310.15	2452.22	28.959	95.22	-0.572
320.15	2530.78	53.878	174.29	-1.919
330.15	2600.37	79.543	253.22	-4.057
340.15	2661.86	105.859	331.74	-6.981
350.15	2720.76	132.773	409.71	-10.689
360.15	2780.60	160.278	487.16	-15.173
370.15	2842.19	188.391	564.15	-20.430
380.15	2905.05	217.127	640.75	-26.454
390.15	2968.53	246.495	717.00	-33.243
400.15	3032.30	276.499	792.93	-40.792
410.15	3096.15	307.142	868.56	-49.100
420.15	3159.89	338.423	943.91	-58.162
430.15	3223.64	370.340	1018.99	-67.976
440.15	3288.33	402.899	1093.81	-78.540
450.15	3354.85	436.114	1168.42	-89.851
460.15	3418.67	469.990	1242.85	-101.907