

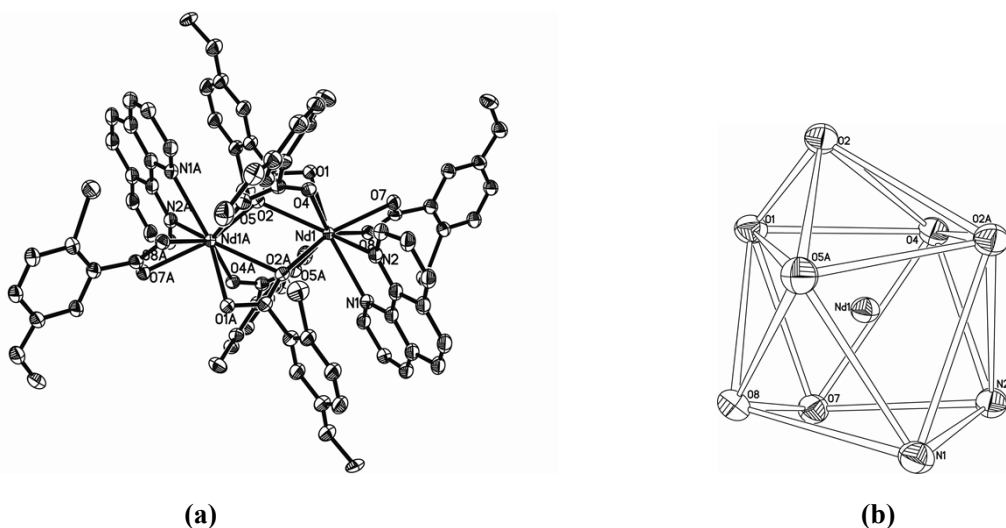


Fig. 1S The crystal structure of complex **1**(a) and coordination geometry of the Nd(III) ion (b) with non-hydrogen atoms drawn by diamond.

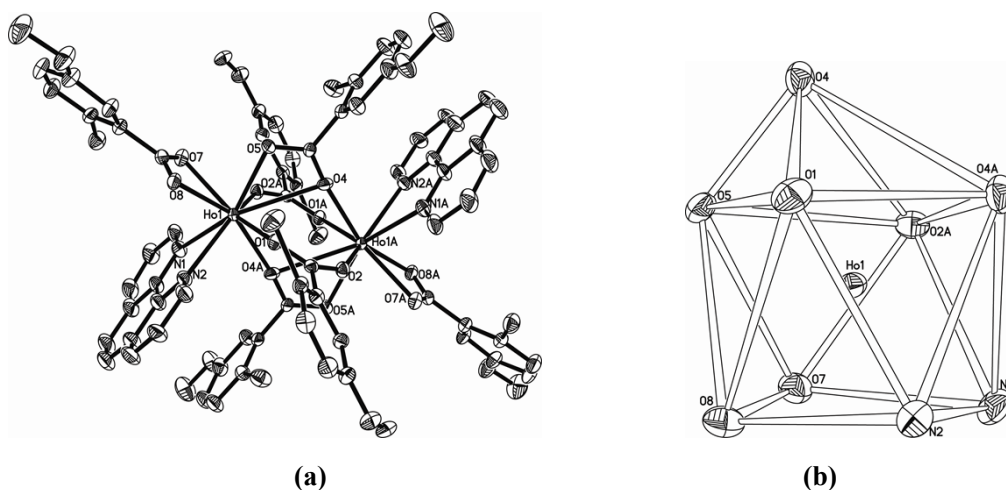


Fig. 2S The crystal structure of complex **3**(a) and coordination geometry of the Ho(III) ion (b) with non-hydrogen atoms drawn by diamond.

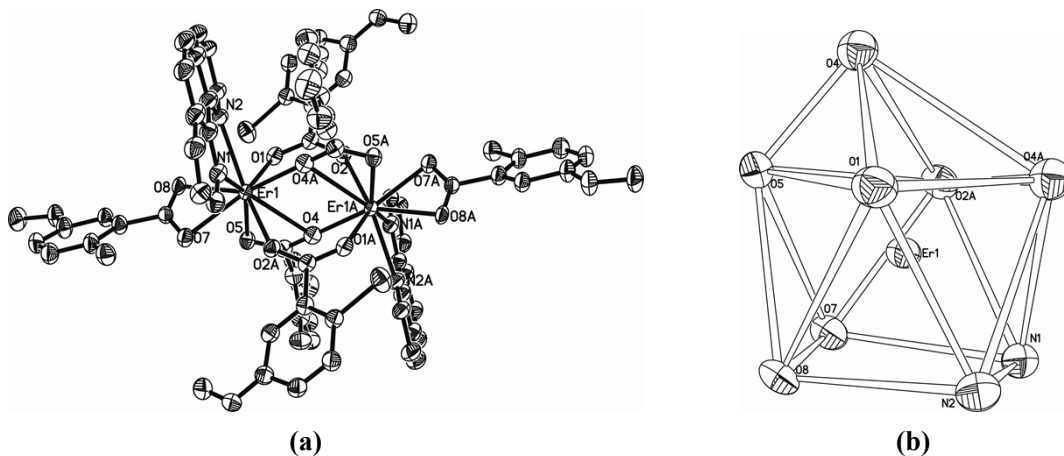


Fig. 3S The crystal structure of complex **4**(a) and coordination geometry of the Er(III) ion (b) with non-hydrogen atoms drawn by diamond.

Table S1 The average molar heat capacity value of the complexes 1 to 2 at normal pressure

T/K	$C_{p,m}/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$	$C_{p,m}/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$	T/K	$C_{p,m}/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$	$C_{p,m}/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$
Complex 1			Complex 2		
263.15	708.95	795.89	360.65	969.07	1101.73
265.65	715.54	804.46	363.15	974.22	1106.55
268.15	721.61	812.26	365.65	983.04	1111.03
270.65	728.16	821.36	368.15	992.44	1117.37
273.15	735.36	830.88	370.65	1005.93	1124.54
275.65	742.55	841.29	373.15	1030.27	1132.58
278.15	749.41	852.03	375.65	1081.97	1142.03
280.65	756.40	861.84	378.15	1114.86	1151.80
283.15	765.05	872.42	380.65	1081.52	1171.45
285.65	773.38	883.30	383.15	1044.02	1227.63
288.15	781.37	894.29	385.65	1032.23	1311.26
290.65	788.99	905.88	388.15	1030.76	1297.11
293.15	797.33	917.38	390.65	1033.96	1226.38
295.65	805.87	928.80	393.15	1038.27	1204.88
298.15	815.02	939.45	395.65	1043.67	1203.08
300.65	824.45	948.60	398.15	1049.57	1206.09
303.15	832.27	956.30	400.65	1056.02	1210.65
305.65	839.96	963.17	403.15	1061.62	1216.08
308.15	847.73	969.21	405.65	1067.67	1220.95
310.65	854.80	973.46	408.15	1073.90	1226.64
313.15	862.22	978.36	410.65	1081.15	1232.43
315.65	867.40	982.54	413.15	1089.63	1238.75
318.15	872.66	987.34	415.65	1099.67	1245.39
320.65	879.20	993.02	418.15	1123.09	1251.40
323.15	887.25	998.84	420.65	1171.00	1257.43
325.65	896.73	1006.14	423.15	1171.98	1264.79
328.15	904.59	1013.93	425.65	1145.27	1272.17
330.65	910.06	1024.18	428.15	1135.98	1278.32
333.15	913.49	1035.57	430.65	1134.53	1284.38
335.65	917.87	1049.16	433.15	1136.13	1292.46
338.15	921.96	1070.20	435.65	1139.06	1300.17
340.65	925.54	1111.25	438.15	1142.72	1308.54
343.15	931.39	1184.68	440.65	1147.52	1314.42
345.65	936.45	1195.20	443.15	1152.76	1320.02
348.15	942.23	1126.76	445.65	1158.37	1327.14
350.65	948.04	1101.00	448.15	1162.63	1334.18
353.15	953.32	1096.10	450.65	1167.29	1340.71
355.65	958.89	1096.22	453.15	1172.85	1347.99
358.15	964.03	1098.61	455.65	1178.26	1357.25

Standard uncertainties u are $u(T)=0.01\text{K}$, $u(C_{p,m})=0.01\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.

Table S2 The average molar heat capacity value of the complexes 3 to 4 at normal pressure

T/K	$C_{p,m}/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$	$C_{p,m}/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$	T/K	$C_{p,m}/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$	$C_{p,m}/(\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1})$
Complex 3			Complex 4		
263.15	538.62	740.95	360.65	784.32	1195.62
265.65	545.20	751.65	363.15	789.66	1199.59
268.15	553.46	761.85	365.65	795.36	1203.64
270.65	561.32	772.28	368.15	801.39	1206.91
273.15	569.48	783.50	370.65	808.25	1210.66
275.65	577.89	794.48	373.15	812.54	1215.20
278.15	586.34	805.63	375.65	819.36	1218.70
280.65	597.16	817.24	378.15	825.44	1220.78
283.15	606.46	830.74	380.65	831.76	1223.89
285.65	615.46	844.48	383.15	837.96	1225.73
288.15	625.40	858.16	385.65	843.99	1227.78
290.65	634.08	872.94	388.15	849.06	1231.35
293.15	642.31	889.66	390.65	854.65	1235.22
295.65	649.68	906.95	393.15	861.29	1239.13
298.15	655.68	924.39	395.65	867.74	1244.06
300.65	662.28	943.10	398.15	873.90	1249.49
303.15	667.29	960.45	400.65	883.55	1254.60
305.65	670.22	975.70	403.15	892.54	1260.13
308.15	672.83	991.95	405.65	900.11	1264.98
310.65	677.85	1009.39	408.15	907.58	1269.79
313.15	682.43	1026.36	410.65	916.37	1276.32
315.65	687.17	1043.75	413.15	923.39	1282.78
318.15	693.23	1062.37	415.65	931.59	1288.68
320.65	699.58	1080.36	418.15	939.06	1295.39
323.15	704.29	1095.64	420.65	945.04	1302.47
325.65	709.70	1107.71	423.15	951.01	1309.01
328.15	715.65	1117.49	425.65	957.91	1314.21
330.65	722.66	1127.91	428.15	963.65	1319.39
333.15	728.67	1138.63	430.65	968.70	1323.58
335.65	735.37	1149.72	433.15	973.35	1327.76
338.15	739.04	1155.41	435.65	977.84	1333.64
340.65	741.66	1160.45	438.15	982.61	1337.93
343.15	745.08	1165.38	440.65	987.76	1342.40
345.65	749.85	1173.71	443.15	991.36	1346.65
348.15	756.63	1180.45	445.65	995.63	1352.04
350.65	762.54	1184.24	448.15	999.92	1357.49
353.15	767.22	1188.09	450.65	1004.11	1363.18
355.65	773.88	1190.78	453.15	1008.24	1370.27
358.15	779.84	1193.54	455.65	1014.05	1377.07

Standard uncertainties u are $u(T)=0.01\text{K}$, $u(C_{p,m})=0.01\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.