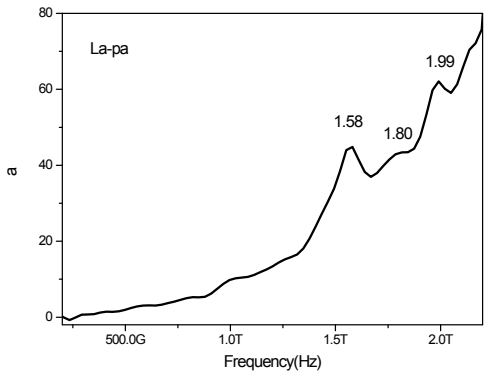
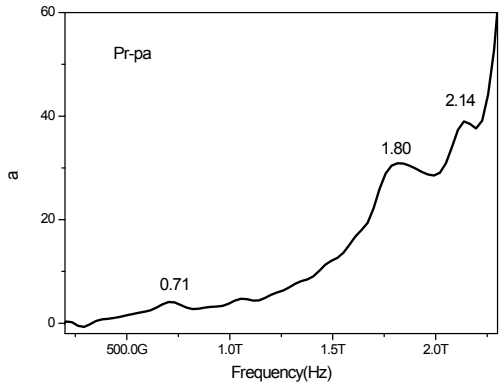
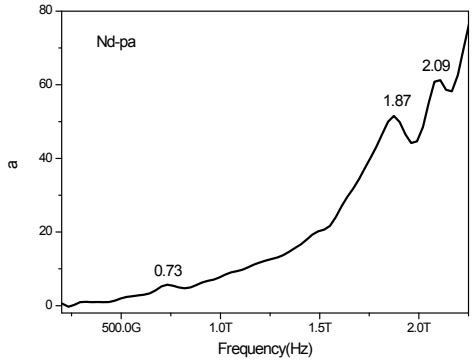
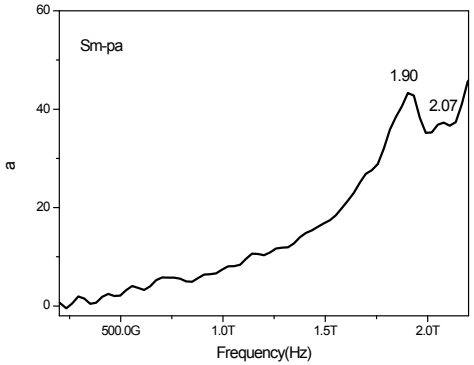
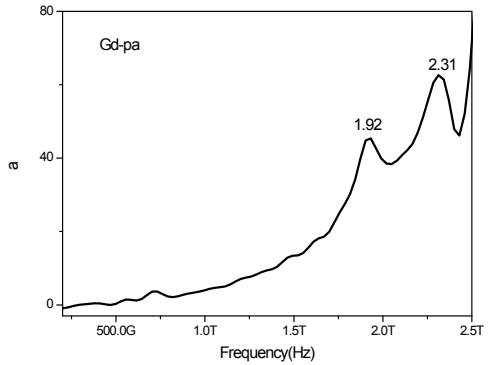
Electronic Supplementary Material (ESI) for CrystEngComm.

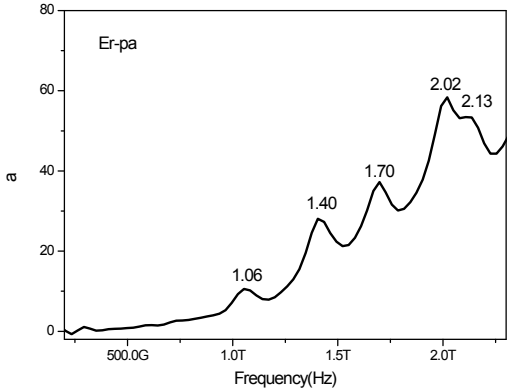












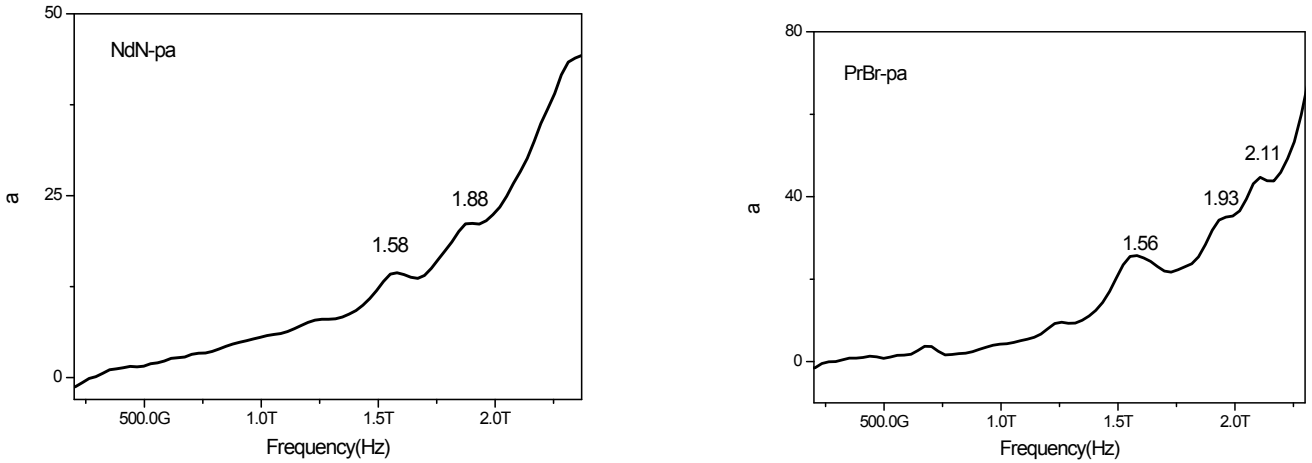


Fig. S1. The THz spectra of eight lanthanide-pa complexes

Table S1 The selected bond lengths (Å) and bond angles (°) in the lanthanide-pa complexes

La-pa		Pr-pa		Nd-pa	
La1–O1	2.451(4)	Pr1–O2	2.424(3)	Nd1–O1	2.4043(19)
La1–O2	2.471(4)	Pr1–O1	2.436(3)	Nd1–O2	2.426(2)
La1–O5	2.513(4)	Pr1–O4	2.481(3)	Nd1–O6	2.4614(19)
La1–O4	2.530(4)	Pr1–O6	2.501(3)	Nd1–O3	2.475(2)
La1–O3	2.558(4)	Pr1–O7	2.518(3)	Nd1–O5	2.500(2)
La1–O7	2.560(4)	Pr1–O3	2.537(3)	Nd1–O7	2.5121(19)
La1–O6	2.573(4)	Pr1–O5	2.542(3)	Nd1–O4	2.531(2)
La1–N1	2.717(5)	Pr1–N3	2.671(3)	Nd1–N1	2.657(2)
La1–N3	2.760(5)	Pr1–N1	2.702(4)	Nd1–N3	2.683(2)
C11–N3–C7	118.0(5)	C5–N1–C1	117.1(4)	C11–N3–C7	117.3(2)
C5–N1–C1	117.4(5)	C7–N3–C11	117.8(4)	C5–N1–C1	117.4(2)
O1–C6–N2	121.7(6)	O2–C12–N4	121.4(4)	N1–C5–C4	123.1(3)
O1–C6–C1	118.9(5)	O2–C12–C7	118.5(4)	O2–C12–N4	121.8(3)
N2–C6–C1	119.4(5)	N4–C12–C7	120.1(4)	O2–C12–C7	118.7(2)
N1–C1–C2	122.9(5)	O1–C6–N2	122.3(4)	N4–C12–C7	119.4(2)
N1–C1–C6	112.9(5)	O1–C6–C1	119.0(4)	N3–C7–C8	122.8(3)
C2–C1–C6	124.2(5)	N2–C6–C1	118.8(4)	N3–C7–C12	113.3(2)
O2–C12–N4	122.2(6)	N3–C7–C8	123.1(4)	C8–C7–C12	123.9(2)
O2–C12–C7	118.9(5)	N3–C7–C12	113.3(4)	N1–C1–C2	123.0(2)
N4–C12–C7	118.9(5)	C8–C7–C12	123.5(4)	N1–C1–C6	112.9(2)
N3–C7–C8	122.6(6)	N1–C1–C2	123.1(4)	C2–C1–C6	124.2(2)
N3–C7–C12	113.5(5)	N1–C1–C6	112.5(4)	C1–C2–C3	118.5(3)
C8–C7–C12	123.9(5)	C2–C1–C6	124.4(4)	C9–C10–C11	118.4(3)
N3–C11–C10	123.2(6)	N3–C11–C10	122.4(5)	O1–C6–N2	121.6(3)

C7–C8–C9	118.8(6)	N1–C5–C4	123.9(4)	O1–C6–C1	118.6(2)
N1–C5–C4	123.1(5)	C1–C2–C3	118.8(4)	N2–C6–C1	119.8(2)
C5–C4–C3	119.3(6)	C9–C10–C11	119.7(4)	C3–C4–C5	119.0(3)
C1–C2–C3	118.8(5)	C7–C8–C9	118.3(4)	C9–C8–C7	119.0(3)
C10–C9–C8	119.0(6)	C2–C3–C4	118.8(5)	N3–C11–C10	123.6(3)
C4–C3–C2	118.2(6)	C10–C9–-C8	118.7(4)	C8–C9–C10	118.8(3)
C9–C10–C11	118.4(6)	C5–C4–C3	118.2(4)	C4–C3–C2	118.9(3)
C5–N1–C1–C2	4.6(8)	C11–N3–C7–C8	3.6(6)	C1–N1–C5–C4	2.8(4)
C5–N1–C1–C6	-176.1(5)	C11–N3–C7–C12	-176.3(4)	C11–N3–C7–C8	-3.8(4)
O1–C6–C1–N1	-0.9(8)	O2–C12–C7–N3	-2.1(6)	C11–N3–C7–C12	174.8(2)
N2–C6–C1–N1	178.1(5)	N4–C12–C7–N3	177.5(4)	O2–C12–C7–N3	1.9(3)
O1–C6–C1–C2	178.4(6)	O2–C12–C7–C8	178.0(4)	N4–C12–C7–N3	-176.9(2)
N2–C6–C1–C2	-2.6(9)	N4–C12–C7–C8	-2.4(6)	O2–C12–C7–C8	-179.6(3)
C11–N3–C7–C8	2.7(9)	C5–N1–C1–C2	3.1(6)	N4–C12–C7–C8	1.6(4)
C11–N3–C7–C12	-175.4(5)	C5–N1–C1–C6	-174.7(4)	C5–N1–C1–C2	-3.8(4)
O2–C12–C7–N3	-1.6(8)	O1–C6–C1–N1	-2.4(6)	C5–N1–C1–C6	176.3(2)
N4–C12–C7–N3	176.8(5)	N2–C6–C1–N1	176.7(4)	N1–C1–C2–C3	1.3(4)
O2–C12–C7–C8	-179.7(6)	O1–C6–C1–C2	179.8(4)	C6–C1–C2–C3	-178.8(2)
N4–C12–C7–C8	-1.3(9)	N2–C6–C1–C2	-1.1(7)	N1–C1–C6–O1	2.1(3)
C7–N3–C11–C10	-0.4(9)	C7–N3–C11–C10	-2.4(6)	C2–C1–C6–O1	-177.8(2)
N3–C7–C8–C9	-1.5(9)	C1–N1–C5–C4	-1.2(7)	N1–C1–C6–N2	-177.2(2)
C12–C7–C8–C9	176.4(6)	N1–C1–C2–C3	-1.3(7)	C2–C1–C6–N2	2.9(4)
C1–N1–C5–C4	-3.6(9)	C6–C1–C2–C3	176.2(4)	N1–C5–C4–C3	0.8(4)
N1–C5–C4–C3	0.0(10)	N3–C11–C10–C9	-0.9(7)	N3–C7–C8–C9	1.7(4)
N1–C1–C2–C3	-1.9(9)	N3–C7–C8–C9	-1.3(6)	C12–C7–C8–C9	-176.6(3)
C6–C1–C2–C3	178.8(6)	C12–C7–C8–C9	178.5(4)	C7–N3–C11–C10	2.3(4)
C7–C8–C9–C10	-2.1(9)	C1–C2–C3–C4	-2.4(7)	C9–C10–C11–N3	1.1(5)

C5–C4–C3–C2	2.7(9)	C11–C10–C9–C8	3.1(7)	C7–C8–C9–C10	1.8(4)
C1–C2–C3–C4	-1.8(9)	C7–C8–C9–C10	-2.1(7)	C11–C10–C9–C8	-3.2(4)
C8–C9–C10–C11	4.3(9)	N1–C5–C4–C3	-2.4(7)	C5–C4–C3–C2	-3.4(4)
N3–C11–C10–C9	-3.2(10)	C2–C3–C4–C5	4.1(7)	C1–C2–C3–C4	2.4(4)

Sm-pa		Eu-pa		Gd-pa	
Sm1–O1	2.370(7)	Eu1–O2	2.371(3)	Gd1–O2	2.362(3)
Sm1–O2	2.396(7)	Eu1–O1	2.393(3)	Gd1–O1	2.390(4)
Sm1–O6	2.437(8)	Eu1–O5	2.424(3)	Gd1–O7	2.411(3)
Sm1–O4	2.439(8)	Eu1–O6	2.438(3)	Gd1–O4	2.421(3)
Sm1–O7	2.468(8)	Eu1–O7	2.455(3)	Gd1–O6	2.448(4)
Sm1–O3	2.492(7)	Eu1–O3	2.472(3)	Gd1–O5	2.458(3)
Sm1–O5	2.520(7)	Eu1–O4	2.497(4)	Gd1–O3	2.487(4)
Sm1–N1	2.618(9)	Eu1–N3	2.615(4)	Gd1–N3	2.606(4)
Sm1–N3	2.654(9)	Eu1–N1	2.644(4)	Gd1–N1	2.631(4)
C7–N3–C11	117.1(9)	C5–N1–C1	117.5(4)	C5–N1–C1	116.6(4)
C5–N1–C1	117.4(9)	C11–N3–C7	117.3(4)	N3–C11–C10	123.6(5)
O2–C12–N4	123.0(10)	O1–C6–N2	121.7(4)	O1–C6–N2	121.5(5)
O2–C12–C7	118.8(9)	O1–C6–C1	118.9(4)	O1–C6–C1	119.4(4)
N4–C12–C7	118.1(9)	N2–C6–C1	119.3(4)	N2–C6–C1	119.1(5)
O1–C6–N2	123.0(11)	O2–C12–N4	121.9(4)	N1–C1–C2	122.9(5)
O1–C6–C1	118.3(10)	O2–C12–C7	118.6(4)	N1–C1–C6	112.8(4)
N2–C6–C1	118.7(9)	N4–C12–C7	119.5(4)	C2–C1–C6	124.3(4)
N1–C1–C2	122.6(10)	N3–C7–C8	123.0(4)	C11–N3–C7	117.4(4)
N1–C1–C6	112.7(9)	N3–C7–C12	112.6(4)	C3–C2–C1	118.7(5)
C2–C1–C6	124.6(9)	C8–C7–C12	124.4(4)	N3–C7–C8	122.3(4)
N3–C7–C8	122.3(10)	N1–C1–C2	122.6(4)	N3–C7–C12	113.3(4)

N3–C7–C12	112.7(9)	N1–C1–C6	113.3(4)	C8–C7–C12	124.4(4)
C8–C7–C12	124.9(10)	C2–C1–C6	124.1(4)	O2–C12–N4	122.0(5)
C3–C2–C1	119.1(10)	C3–C2–C1	118.7(4)	O2–C12–C7	118.1(5)
C9–C8–C7	120.2(10)	N3–C11–C10	123.2(4)	N4–C12–C7	120.0(5)
N1–C5–C4	123.0(10)	N1–C5–C4	123.9(4)	C9–C10–C11	118.6(5)
C8–C9–C10	118.4(10)	C7–C8–C9	118.7(4)	N1–C5–C4	123.8(5)
C3–C4–C5	118.8(10)	C2–C3–C4	119.1(4)	C3–C4–C5	119.0(5)
N3–C11–C10	123.8(10)	C9–C10–C11	118.9(4)	C9–C8–C7	118.8(5)
C9–C10–C11	117.9(11)	C10–C9–C8	118.8(4)	C4–C3–C2	118.8(5)
C4–C3–C2	118.8(10)	C5–C4-C3	118.2(4)	C10–C9–C8	119.1(5)
C5–N1–C1–C2	3.9(15)	C11–N3–C7–C8	3.7(6)	C5–N1–C1–C6	175.4(4)
C5–N1–C1–C6	-176.6(9)	C11–N3–C7–C12	-175.6(4)	O1–C6–C1–N1	1.4(6)
O2–C6–C1–N1	-2.0(14)	O2–C12–C7–N3	-3.3(6)	N2–C6–C1–N1	-175.7(4)
N2–C6–C1–N1	176.6(10)	N4–C12–C7–N3	176.5(4)	O1–C6–C1–C2	-179.5(5)
O1–C6–C1–C2	177.5(10)	O2–C12–C7–C8	177.4(4)	N2–C6–C1–C2	3.5(7)
N2–C6–C1–C2	-3.8(16)	N4–C12–C7–C8	-2.8(7)	C10–C11–N3–C7	1.9(7)
C11–N3–C7–C8	3.9(15)	C5–N1–C1–C2	4.3(7)	C10–C11–N3–Gd1	-173.1(4)
C11–N3–C7–C12	-174.7(9)	C5–N1–C1–C6	-175.0(4)	N1–C1–C2–C3	2.0(7)
O2–C12–C7–N3	-1.8(14)	O1–C6–C1–N1	-1.3(6)	C6–C1–C2–C3	-177.1(5)
N4–C12–C7–N3	176.5(10)	N2–C6–C1–N1	176.0(4)	C11–N3–C7–C8	-3.1(7)
O2–C12–C7–C8	179.6(10)	O1–C6–C1–C2	179.5(4)	C11–N3–C7–C12	176.0(4)
N4–C12–C7–C8	-2.1(16)	N2–C6–C1–C2	-3.2(7)	N3–C7–C12–O2	3.3(6)
N1–C1-C2–C3	-0.7(16)	N1–C1–C2–C3	-2.4(7)	C8–C7–C12–O2	-177.5(5)
C6–C1–C2–C3	179.8(10)	C6–C1–C2–C3	176.8(4)	N3–C7–C12–N4	-176.4(4)
N3–C7–C8–C9	-1.9(16)	C7–N3–C11–C10	-2.9(7)	C8–C7–C12–N4	2.8(7)
C12–C7–C8–C9	176.6(10)	C1–N1–C5–C4	-2.2(7)	N3–C11–C10–C9	1.9(8)
C1–N1–C5–C4	-3.1(16)	N3–C7–C8–C9	-1.0(7)	C1–N1–C5–C4	2.2(8)

C7–C8–C9–C10	-2.2(17)	C12–C7–C8–C9	178.2(4)	N1–C5–C4–C3	1.4(8)
N1–C5–C4–C3	-0.8(17)	C1–C2–C3–C4	-1.7(7)	N3–C7–C8–C9	0.5(7)
C7–N3–C11–C10	-2.1(17)	N3–C11–C10–C9	-0.7(7)	C12–C7–C8–C9	-178.5(4)
C8–C9–C10–C11	3.9(17)	C11–C10–C9–C8	3.4(7)	C5–C4–C3–C2	-3.3(8)
N3–C11–C10–C9	-1.8(18)	C7–C8–C9–C10	-2.6(7)	C1–C2–C3–C4	1.7(7)
C5–C4–C3–C2	4.0(16)	N1–C5–C4–C3	-1.8(8)	C11–C10–C9–C8	-4.5(7)
C1–C2–C3–C4	-3.3(16)	C2–C3–C4–C5	3.7(7)	C7–C8–C9–C10	3.4(7)

Tb-pa		Er-pa		$PrBr_3$-pa	
Tb1–O2	2.343(6)	Er1–O2	2.263(2)	Pr1–O1	2.421(7)
Tb1–O1	2.356(6)	Er1–O1	2.268(2)	Pr1–O2	2.432(7)
Tb1–O5	2.401(6)	Er1–O3	2.332(2)	Pr1–O6	2.486(7)
Tb1–O7	2.406(7)	Er1–O5	2.337(3)	Pr1–O5	2.492(7)
Tb1–O6	2.421(7)	Er1–O4	2.367(3)	Pr1–O7	2.520(8)
Tb1–O3	2.449(6)	Er1–O6	2.376(2)	Pr1–O3	2.525(7)
Tb1–O4	2.496(6)	Er1–N3	2.498(3)	Pr1–O4	2.566(7)
Tb1–N3	2.581(7)	Er1–N1	2.514(3)	Pr1–N3	2.709(7)
Tb1–N1	2.618(8)			Pr1–N1	2.725(8)
C5–N1–C1	117.9(8)	C5–N1–C1	117.8(3)	C11–N3–C7	119.7(8)
C11–N3–C7	117.8(8)	C11–N3–C7	117.6(3)	C5–N1–C1	117.2(9)
O2–C12–N4	123.0(8)	N1–C5–C4	122.4(3)	O1–C6–N2	121.5(10)
O2–C12–C7	117.6(8)	N1–C1–C2	122.7(3)	O1–C6–C1	119.5(8)
N4–C12–C7	119.3(8)	N1–C1–C6	113.0(3)	N2–C6–C1	119.0(9)
O1–C6–N2	122.9(8)	C2–C1–C6	124.3(3)	N3–C11–C10	120.8(10)
O1–C6–C1	118.7(8)	N3–C7–C8	123.2(3)	N3–C7–C8	121.4(9)
N2–C6–C1	118.4(8)	N3–C7–C12	112.7(3)	N3–C7–C12	114.3(8)
N3–C7–C8	122.2(8)	C8–C7–C12	124.1(3)	C8–C7–C12	124.2(9)

N3–C7–C12	112.7(7)	O2–C12–N4	122.1(3)	O2–C12–N4	119.5(9)
C8–C7–C12	125.1(8)	O2–C12–C7	118.2(3)	O2–C12–C7	119.1(9)
N1–C1–C2	122.7(8)	N4–C12–C7	119.7(3)	N4–C12–C7	121.4(9)
N1–C1–C6	113.2(8)	C7–C8–C9	118.1(3)	N1–C5–C4	122.2(10)
C2–C1–C6	124.1(8)	C3–C4–C5	119.1(3)	C2–C1–N1	122.1(10)
N3–C11–C10	122.1(9)	C3–C2–C1	119.2(3)	C2–C1–C6	125.6(9)
N1–C5–C4	123.6(9)	O1–C6–N2	120.7(3)	N1–C1–C6	112.3(8)
C3–C2–C1	118.0(9)	O1–C6–C1	118.9(3)	C9–C10–C11	119.7(10)
C8–C9–C10	118.3(8)	N2–C6–C1	120.4(3)	C10–C9–C8	119.6(9)
C9–C8–C7	120.1(9)	N3–C11–C10	122.8(3)	C9–C8–C7	118.5(10)
C9–C10–C11	119.1(8)	C10–C9–C8	119.6(3)	C4–C3–C2	118.5(11)
C2–C3–C4	119.5(9)	C9–C10–C11	118.6(3)	C1–C2–C3	120.2(11)
C3–C4–C5	118.1(9)	C2–C3–C4	118.8(3)	C3–C4–C5	119.7(11)
C11–N3–C7–C8	4.8(13)	C1–N1–C5–C4	-0.3(5)	C7–N3–C11–C10	0.9(16)
C11–N3–C7–C12	-175.8(8)	C5–N1–C1–C2	-1.6(5)	C11–N3–C7–C8	-2.0(15)
O2–C12–C7–N3	-1.6(12)	C5–N1–C1–C6	177.9(3)	C11–N3–C7–C12	174.5(9)
N4–C12–C7–N3	176.2(8)	C11–N3–C7–C8	0.7(5)	N3–C7–C12–O2	5.3(13)
O2–C12–C7–C8	177.7(9)	C11–N3–C7–C12	-177.3(3)	C8–C7–C12–O2	-178.3(10)
N4–C12–C7–C8	-4.4(14)	N3–C7–C12–O2	6.5(4)	N3–C7–C12–N4	-174.7(10)
C5–N1–C1–C2	5.7(14)	C8–C7–C12–O2	-171.5(3)	C8–C7–C12–N4	1.7(16)
C5–N1–C1–C6	-174.6(8)	N3–C7–C12-N4	-174.1(3)	C1–N1–C5–C4	1.7(16)
O1–C6–C1–N1	-2.3(12)	C8-C7-C12–N4	7.9(5)	C5–N1–C1–C2	-3.6(15)
N2–C6–C1–N1	176.2(9)	N3–C7–C8–C9	-0.8(5)	C5–N1–C1–C6	174.9(9)
O1–C6–C1–C2	177.4(9)	C12–C7–C8–C9	177.0(3)	O1–C6–C1–C2	-179.8(11)
N2–C6–C1–C2	-4.1(14)	N1–C5–C4–C3	2.2(5)	N2–C6–C1–C2	0.9(17)
C7–N3–C11–C10	-3.5(13)	N1–C1–C2–C3	1.6(5)	O1–C6–C1–N1	1.8(14)
C1–N1–C5–C4	-3.2(14)	C6–C1–C2–C3	-177.9(3)	N2–C6–C1–N1	-177.6(10)

N1–C1–C2–C3	-3.4(14)	N1–C1–C6–O1	7.8(4)	N3–C11–C10–C9	2.5(17)
C6–C1–C2–C3	176.9(9)	C2–C1–C6–O1	-172.7(3)	C11–C10–C9–C8	-4.8(17)
C10–C9–C8–C7	-3.9(14)	N1–C1–C6–N2	-170.3(3)	C10–C9–C8–C7	3.7(16)
N3–C7–C8–C9	-1.1(14)	C2–C1–C6–N2	9.2(5)	N3–C7–C8–C9	-0.3(16)
C12–C7–C8–C9	179.6(9)	C7–N3–C11–C10	0.3(5)	C12–C7–C8–C9	-176.5(10)
C8–C9–C10–C11	5.1(14)	C7–C8–C9–C10	-0.2(5)	N1–C1–C2–C3	2.9(17)
N3–C11–C10–C9	-1.4(14)	C8–C9–C10–C11	1.1(6)	C6–C1–C2–C3	-175.4(10)
C1–C2–C3–C4	-1.4(14)	N3–C11–C10–C9	-1.2(6)	C4–C3–C2–C1	-0.2(18)
C2–C3–C4–C5	3.8(14)	C1–C2–C3–C4	0.4(6)	C2–C3–C4–C5	-1.6(19)
N1–C5–C4–C3	-1.5(15)	C5–C4–C3–C2	-2.2(6)	N1–C5–C4–C3	0.9(19)

NdN-pa

Nd1–O3	2.427(3)				
Nd1–O2	2.439(3)	C5–N1–C1–C2	-1.2(6)	C5–N1–C1	117.4(4)
Nd1–O1	2.458(3)	N1–C1–C2–C3	0.3(7)	C7–N3–C11	117.2(4)
Nd1–O7	2.541(3)	C1–C2–C3–C4	0.3(7)	C13–N5–C17	116.8(4)
Nd1–O5	2.586(3)	C2–C3–C4–C5	-0.2(7)	O6–N7–O4	121.3(4)
Nd1–O8	2.591(3)	C1–N1–C5–C4	1.4(6)	O6–N7–O5	120.4(4)
Nd1–O4	2.641(3)	C1–N1–C5–C6	-179.0(4)	O4–N7–O5	118.3(3)
Nd1–N1	2.664(4)	C3–C4–C5–N1	-0.7(6)	O9–N8–O8	122.2(4)
Nd1–N5	2.678(4)	C3–C4–C5–C6	179.7(4)	O9–N8–O7	121.4(4)
Nd1–N3	2.688(4)	N1–C5–C6–O1	-11.8(5)	O8–N8–O7	116.4(3)
		C4–C5–C6–O1	167.9(4)	C19–N9–C23	116.8(4)
		N1–C5–C6–N2	167.4(4)	C3–C2–C1	119.2(4)
C8–C9–C10–C11	1.7(6)	C4–C5–C6–N2	-13.0(6)	C2–C3–C4	119.0(4)
C7–N3–C11–C10	-2.7(6)	C11–N3–C7–C8	2.8(6)	C5–C4–C3	118.2(4)
C7–N3–C11–C12	178.9(4)	N3–C7–C8–C9	-0.7(7)	N1–C5–C4	123.2(4)
C9–C10–C11–N3	0.5(6)	C7–C8–C9–C10	-1.6(7)	N1–C5–C6	113.4(4)

C9–C10–C11–C12	178.7(4)	N5–C17–C18–N6	164.8(4)	C4–C5–C6	123.4(4)
N3–C11–C12–O2	24.6(5)	C16–C17–C18–N6	-15.8(6)	O1–C6–N2	122.4(4)
C10–C11–C12–O2	-153.7(4)	C23–N9–C19–C20	1.4(7)	O1–C6–C5	118.7(4)
N3–C11–C12–N4	-154.5(4)	N9–C19–C20–C21	-0.5(8)	N2–C6–C5	118.9(4)
C10–C11–C12–N4	27.1(6)	C19–C20–C21–C22	-0.3(8)	N3–C7–C8	122.6(4)
C17–N5–C13–C14	-0.8(6)	C20–C21–C22–C23	0.2(8)	C9–C8–C7	119.1(4)
N5–C13–C14–C15	-1.4(7)	C19–N9–C23–C22	-1.5(7)	C10–C9–C8	118.7(4)
C13–C14–C15–C16	2.7(7)	C19–N9–C23–C24	177.0(4)	C9–C10–C11	118.9(4)
C14–C15–C16–C17	-1.8(7)	C21–C22–C23–N9	0.8(7)	N3–C11–C10	123.3(4)
C13–N5–C17–C16	1.7(6)	C21–C22–C23–C24	-177.6(5)	N3–C11–C12	111.9(3)
C13–N5–C17–C18	-178.9(4)	N9–C23–C24–O10	-162.7(4)	C10–C11–C12	124.7(4)
C15–C16–C17–N5	-0.5(6)	C22–C23–C24–O10	15.8(7)	O2–C12–N4	122.5(4)
C15–C16–C17–C18	-179.8(4)	N9–C23–C24–N10	16.3(6)	O2–C12–C11	119.3(4)
N5–C17–C18–O3	-13.2(5)	C22–C23–C24–N10	-165.2(4)	N4–C12–C11	118.2(4)
C16–C17–C18–O3	166.2(4)			N5–C13–C14	123.8(4)
				C15–C14–C13	118.4(4)
C16–C17–C18	124.2(4)	N6–C18–C17	118.3(4)	C14–C15–C16	119.3(4)
O3–C18–N6	122.3(4)	N9–C19–C20	124.4(5)	C17–C16–C15	118.5(4)
O3–C18–C17	119.4(4)	C19–C20–C21	118.6(5)	N5–C17–C16	123.1(4)
O10–C24–N10	123.1(4)	C20–C21–C22	118.2(5)	N5–C17–C18	112.6(3)
O10–C24–C23	120.4(4)	C23–C22–C21	119.2(5)	N9–C23–C22	122.7(4)
N10–C24–C23	116.6(4)	C22–C23–C24	121.2(4)	N9–C23–C24	116.1(4)

Table S2 The IR bands and possible assignments for lanthanide-pa complexes in the 4000–650 cm^{-1} region

Pa	La	Pr	Nd	Sm	Eu	Gd	Tb	Er	PrBr	NdN	Possible assignments
3420								3469	3380	3384	
	3304	3304	3307	3346	3312	3312	3346	3351	3354	3357	
3277									3299	3288	$\nu(NH_2)$
	3212	3213	3214	3238	3215	3217	3219		3214		
3187	3188	3190	3190		3191	3193		3184	3180	3181	
			3156						3169		
			3143								
3061										3092	ν(CH)
							2925				
							2854				
								2791			
2752	2752	2749						2769			
1662	1665	1665	1665	1666	1666	1667	1667	1681	1660	1675	ν(CO)
			1621	1637	1626	1629	1632	1616	1610	1615	
1605	1613	1613	1613		1614	1614	1616				NH_2scis
1588	1583	1583	1583	1584	1585	1585	1585	1581	1581	1583	νring
1569	1568	1568	1568	1568	1569	1569	1569	1567	1568	1569	νring
1469	1491	1492	1493	1493	1493	1494	1494	1505	1492	1493	δCH
										1482	
				1448			1451	1455	1450	1445	
1444	1434	1435	1436	1436	1436	1437	1438	1433	1434	1432	δCH
1393				1410						1410	ν(CN)
										1346	
										1327	

	1309	1309	1309	1309	1309	1309	1309	1309	1308	1308	
1285										1296	δCH
1254	1260	1261	1261	1261	1261	1261	1261	1264	1260	1259	νring
1226	1221	1222	1222	1222	1223	1223	1224	1225	1217	1223	
		1182	1182	1182	1183	1183	1184	1180		1178	
1166	1163	1164	1164	1164	1165	1165	1165	1159	1164	1158	νring
						1122	1123				
1144	1118	1119	1120	1121	1119	1119	1118	1119	1119	1116	δCH
		1093	1094	1095	1095	1096	1097	1095	1092	1091	δCH
1097	1081	1081	1082	1082	1082	1082	1082		1076	1055	NH2rock
1044	1055	1056	1056	1056	1057	1057	1057	1055	1056	1049	νring
										1040	
997	1009	1010	1011	1011	1012	1012	1012	1013	1009	1009	γ(CH)
										997	νring
										977	
909	907	907	907	907	907	907	907	911	903	910	γ(CH)
										829	
826	820	820	820	820	820	820	820	825	818	816	γ(CH)
797	785	786	787	787	788	788	789	794	784	784	δring
771								786		762	
758	755	756	756	756	757	757	757	758	753	754	τring
										744	
			727					727	720	712	
695						672		691			γ(CO)
649	654	656	658	657	658	659	660	662	656	651	
632	632	633	633	632	633	633	633	634	633	630	
611	612	614	614	616	614	613	614			616	

Table S3 The band positions in the Raman spectra of the lanthanide-pa complexes in the 3700–100 cm^{-1} region

Pa	La	Pr	Nd	Sm	Eu	Gd	Tb	Er	PrBr	NdN
	3363	3375	3302	3386	3308	3296	3296		3380	
	3193			3192	3193			3140		
	3144				3143	3144	3144	3085		
3064	3072	3068	3078	3072	3078	3078	3080	3074	3065	3078
	3063		3063		3063	3064	3066	3059		
	2994				2992	2992	2994			
	2882									
			2110							2185
			2058							2136
			2022							
			1966							1899
			1864							1853
			1784							
1664	1655	1654	1675	1672	1676	1677	1678	1695	1666	
			1644					1644		
	1614	1608	1614	1610	1614	1615	1616	1608	1606	1613
1591			1586		1586	1587	1588			
1572	1572	1572	1574	1571	1574	1574	1575	1570	1572	1573
	1490	1487	1494		1494	1494	1495	1498	1489	
1473				1488				1454	1446	1492
1448	1448	1444	1448	1447	1449	1449	1451	1434	1430	1446
1404	1430	1427	1437	1430	1437	1437	1439			1431
1294	1314	1308	1310	1310	1310	1310	1310	1308	1307	1314
1256		1261	1263		1263	1263	1264	1265	1261	
1170	1183	1176	1184	1181	1184	1184	1186	1182	1179	1177
1154	1163	1160	1167	1164	1166	1167	1167	1161	1160	1160

1146	1125	1111	1122	1118	1123	1123	1124	1123	1113	1116
1089	1092		1095	1084	1096	1096	1097	1096	1087	1093
		1082	1083		1083	1083	1085			
1046	1059	1052	1057	1054	1056	1057	1058	1057	1054	1049
										1041
	1007	1007	1010	1010	1010	1010	1011	1011	1009	1010
999		998						1000		996
989						975		991		
		902	907		907	910	910	910	908	
									857	
826	823	818	821	810	820	820	821	820	817	820
781	781	781	787	782	788	788	790	794	782	785
			758		758	758	760	760		744
								725		711
								665		
641	632	631	633	634	633	633	634	634	632	632
618										615
		505		500	506	506	510	519		
499			441		441	441				
427	426	418	425	423	426	428	430	438	419	419
406						412	413	411		
								361		
					287	278	282	301		
246	287		201	245	201	202	204		272	
197										
180	181			179				186		181
	147				154	158	161	160		
118	120	128	136	124	138	139	141	115	125	126
	108		106		106	105	107			

Table S4 The band positions in the FIR spectra for the lanthanide-pa complexes in the 650–50 cm^{-1} region

Pa	La	Pr	Nd	Sm	Eu	Gd	Tb	Er	PrBr	NdN
649	650									
630	632	632	632	632	632	633	632	633	632	629
609	597	613	613	613	613	613	614		597	618
									552	533
519								521		519
420	427	441	441	440	441	439	441			
	416	419	420	421	422	424	425	424	418	
	403	405	405	406	406	407	407	409	402	409
385								366		
	293	286	286	287	288	291	292	307	296	285
252	249	260	265	271	275				281	
				230	233	237	239			250
	212	218	218	217	217	220	224	220	217	222
										203
							183	190		191
177	186				161	164	168	159	153	153
		142	143	143	143			150	138	129
135	128	133	132			137	137	119		119
	94	102	104	106		94	94	83	93	83
76			63	65	67	67	67	70		
54										

Table S5 The band positions in the THz spectra of the lanthanide-pa complexes (THz)

Pa	La	Pr	Nd	Sm	Eu	Gd	Tb	Er	PrBr	NdN
		0.71	0.73		0.73		0.73			
								1.06		
								1.40	1.56	1.58
	1.58						1.61	1.70		
	1.80	1.80	1.87							1.88
				1.90	1.90	1.92	1.95		1.93	
	1.99	2.14	2.09	2.07			2.14	2.02	2.11	
						2.31		2.13		