Supplementary Information

A series of 3D Lanthanide Coordination Polymers decorated with rigid 3,5-Pyridinedicarboxylic acid linker: Syntheses, Structural diversity, DFT study, Hirshfeld Surface Analysis, Luminescence and Magnetic Properties

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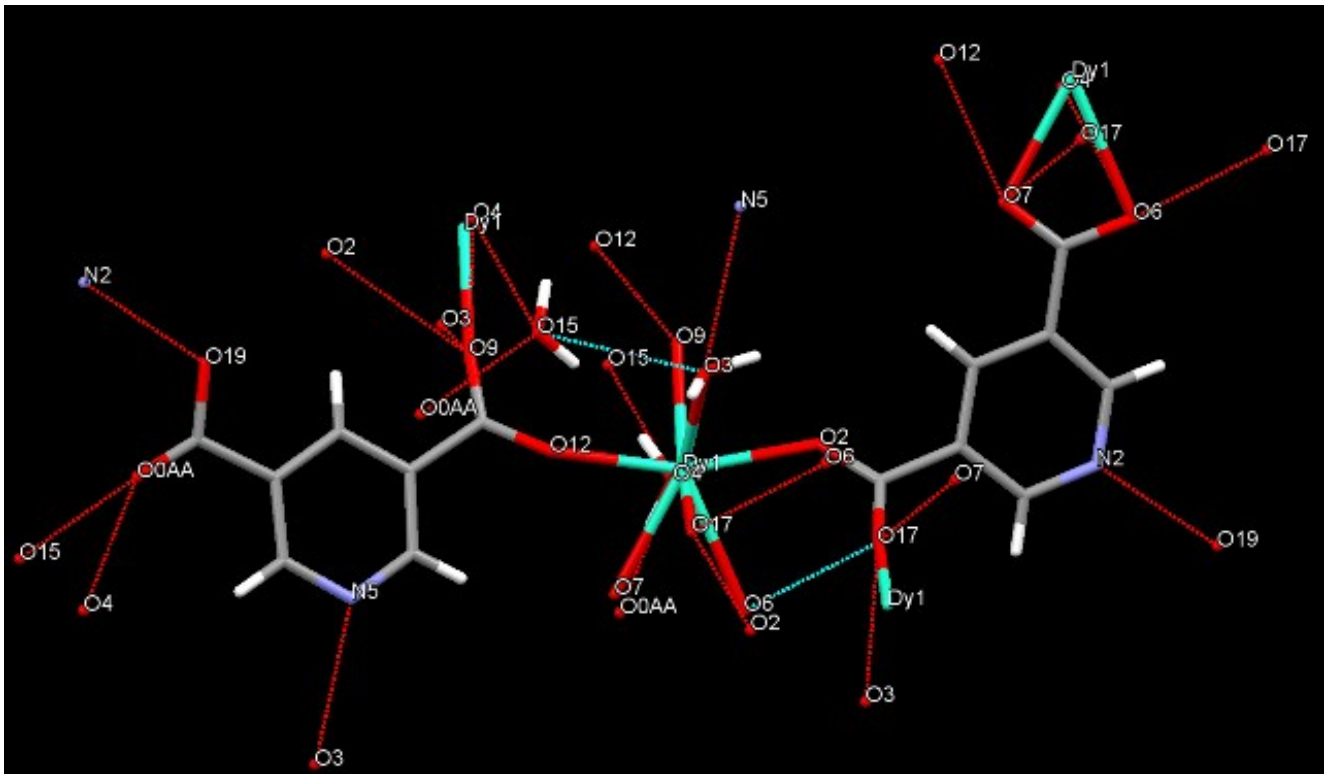

Fig. S1 (a) Number and positions of Hydrogen bonds in asymmetric unit of CP **1**.

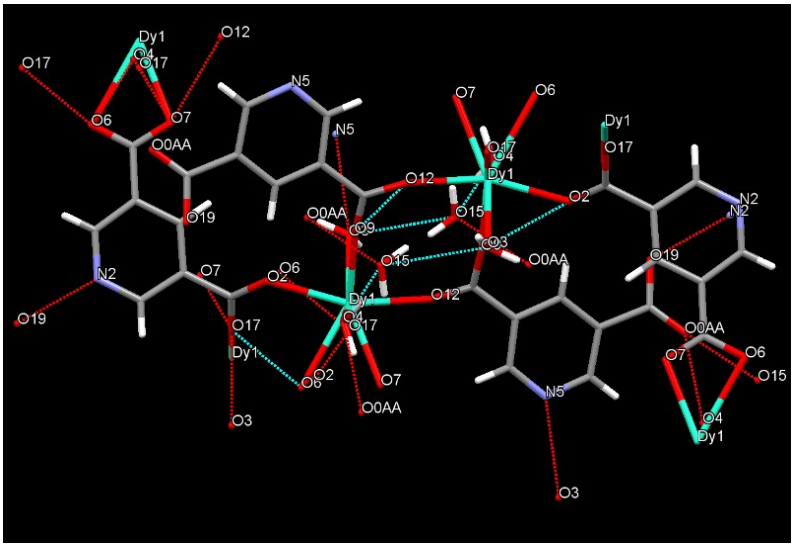

Fig. S1(b). Number and positions of Hydrogen bonds in CP **1**.

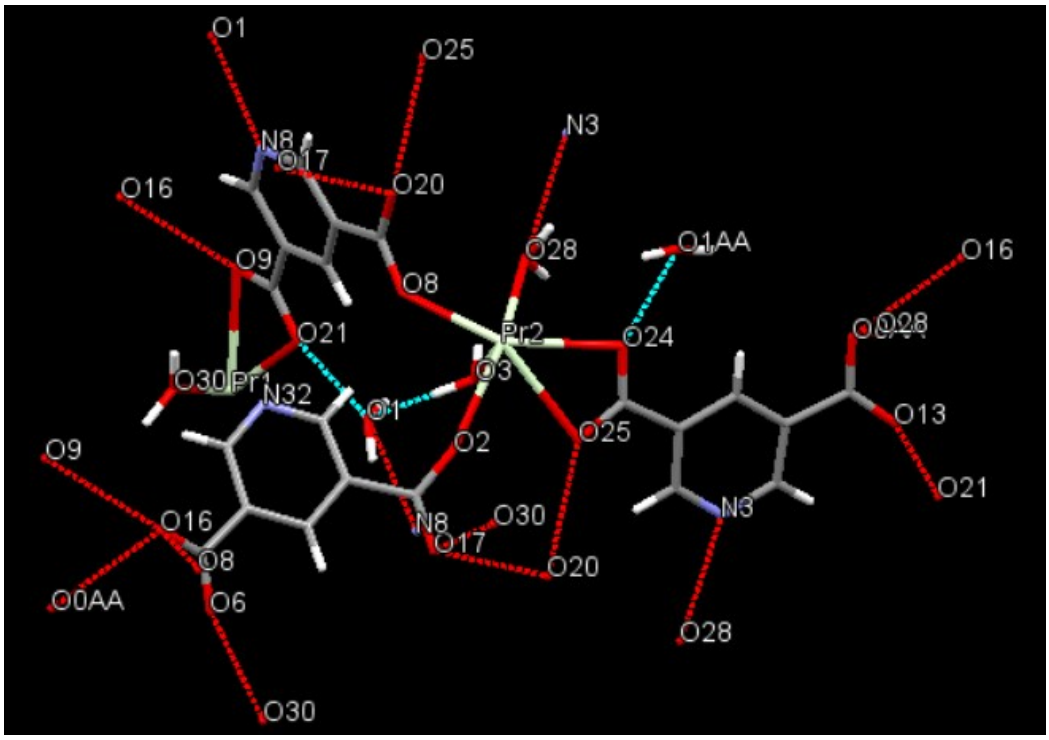

Fig. S2(a) Number and positions of Hydrogen bonds in asymmetric unit of CP **2.**

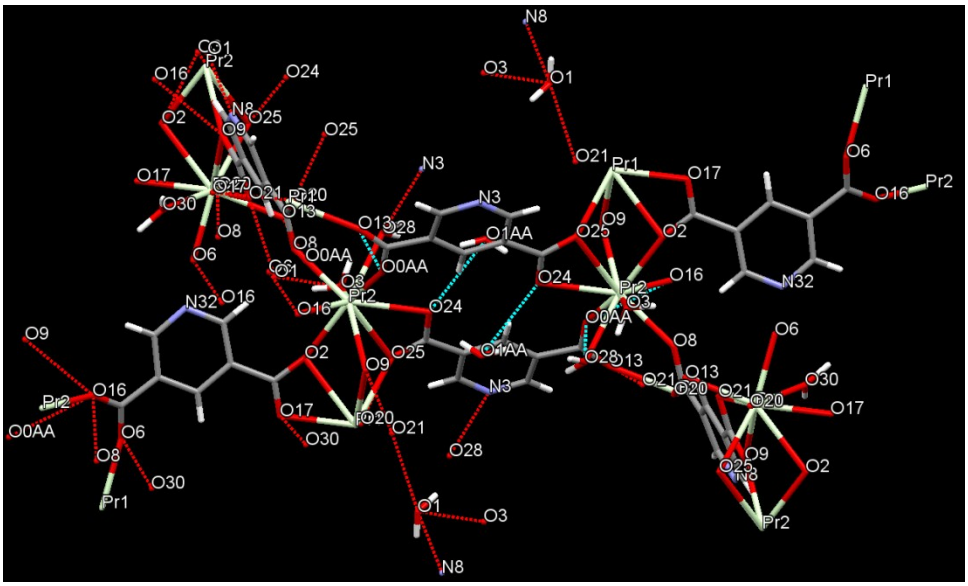

Fig. S2(b). Number and positions of Hydrogen bonds in CP **2**.

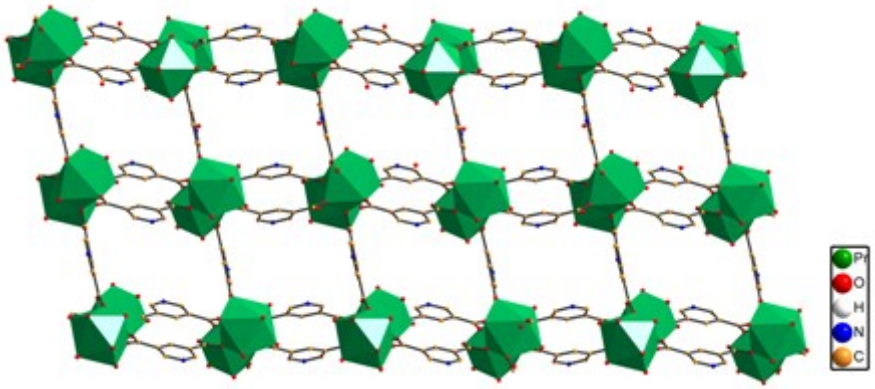

Fig. S2(c) Packing of CP **2** along a-axis.

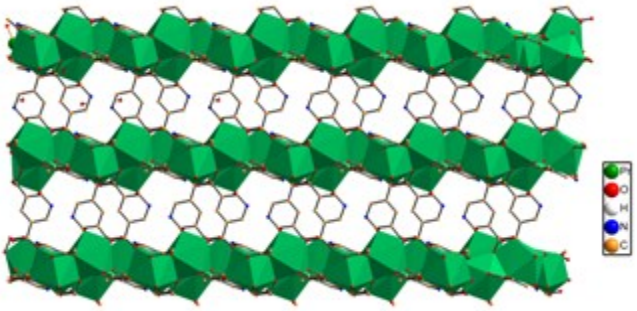

Fig. S2(d) Packing of CP **2** along b-axis.

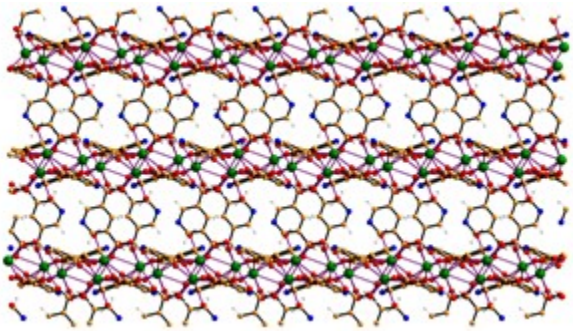

Fig. S2 (e) Packing of CP **2** along c-axis.

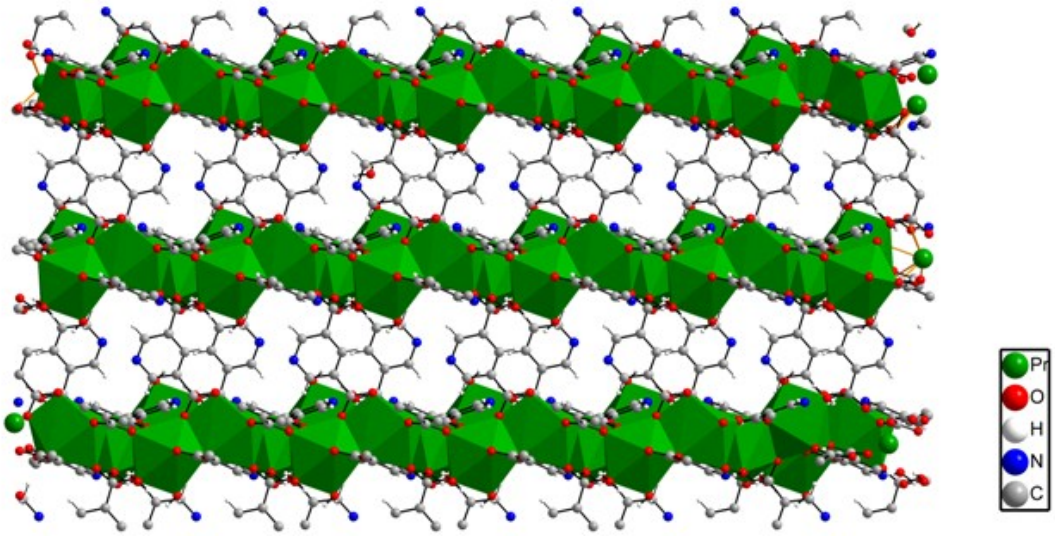

Fig. S2 (f) Packing of CP **2** along c-axis.

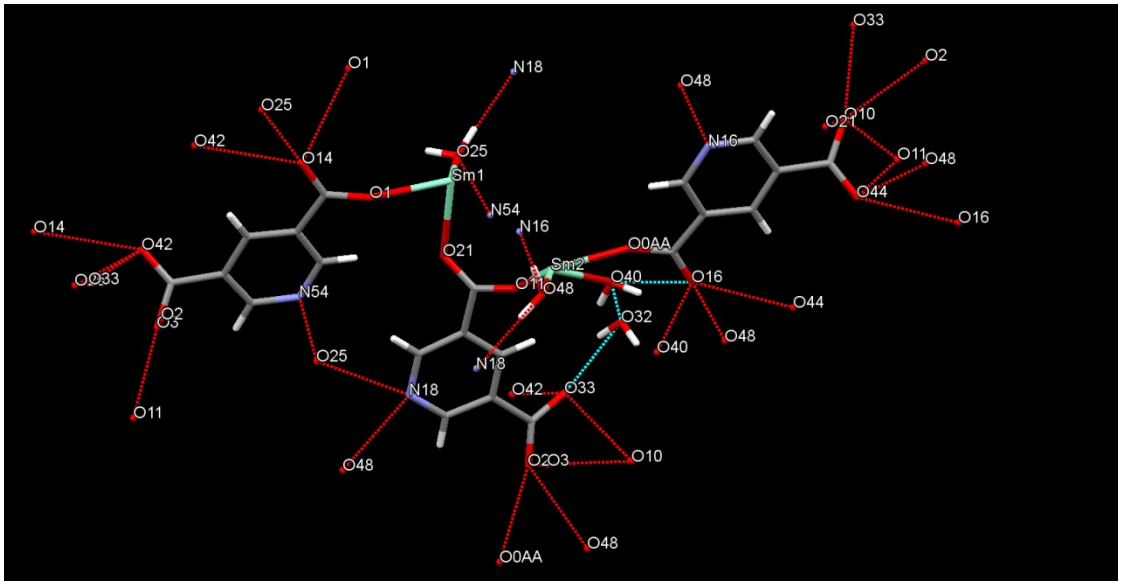

Fig. S3(a) Number and positions of Hydrogen bonds in asymmetric unit of CP **3**.

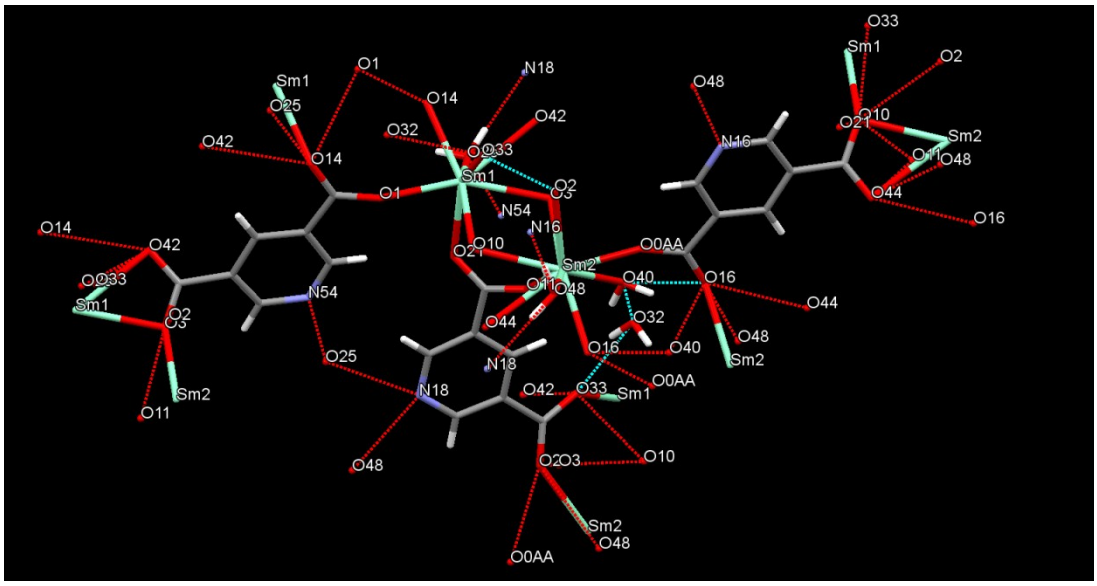

Fig. S3(b) Number and positions of Hydrogen bonds in CP **3**.

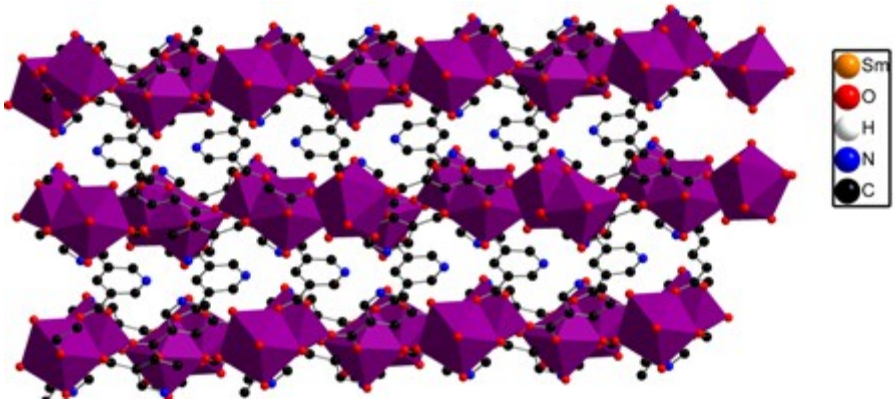

Fig S3 (c) Packing of CP **3** along a-axis.

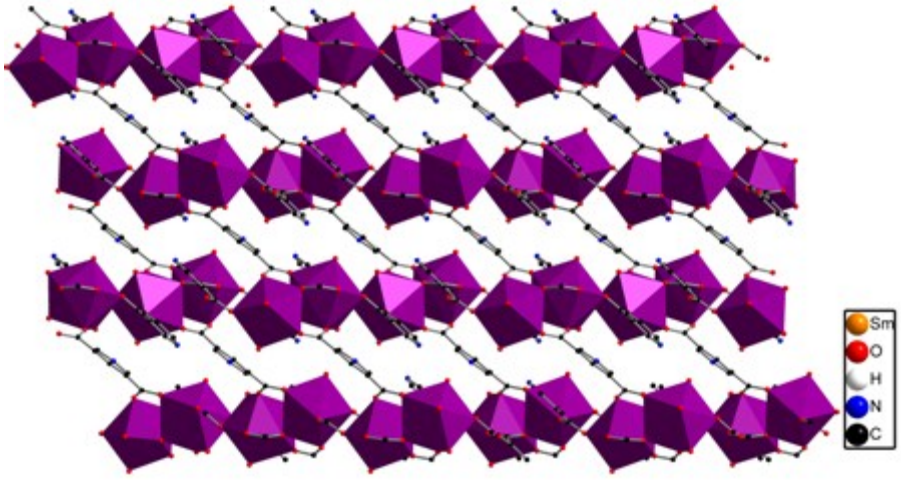

Fig. S3(d) Packing of CP **3** along b-axis.

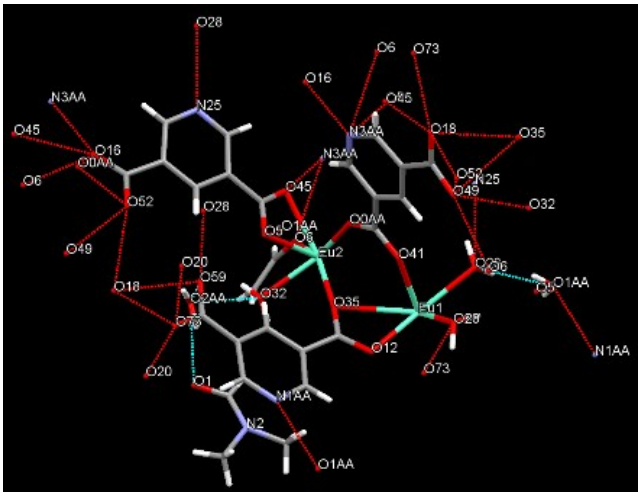

Fig. S4(a) Number and positions of Hydrogen bonds in asymmetric unit of CP **4**.

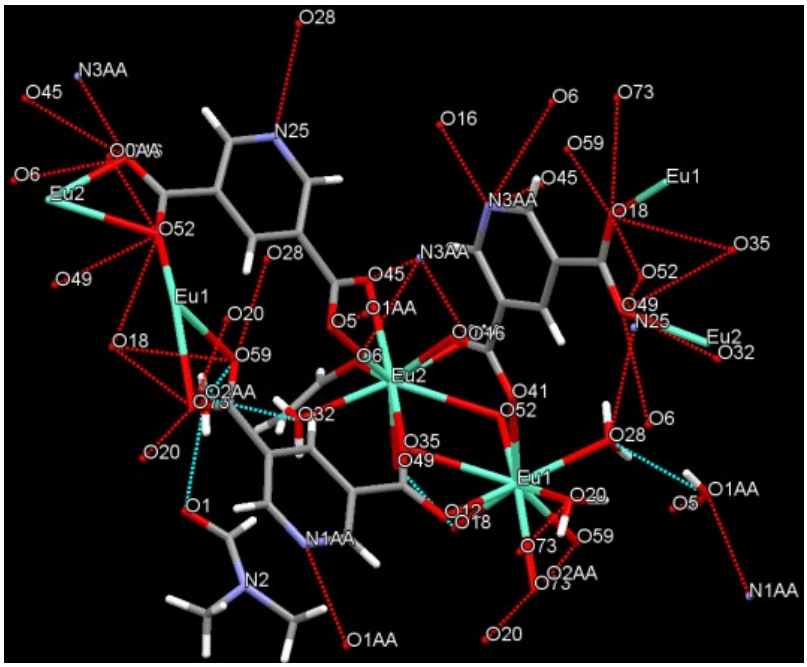

Fig. S4(b) Number and positions of Hydrogen bonds in CP **4**.

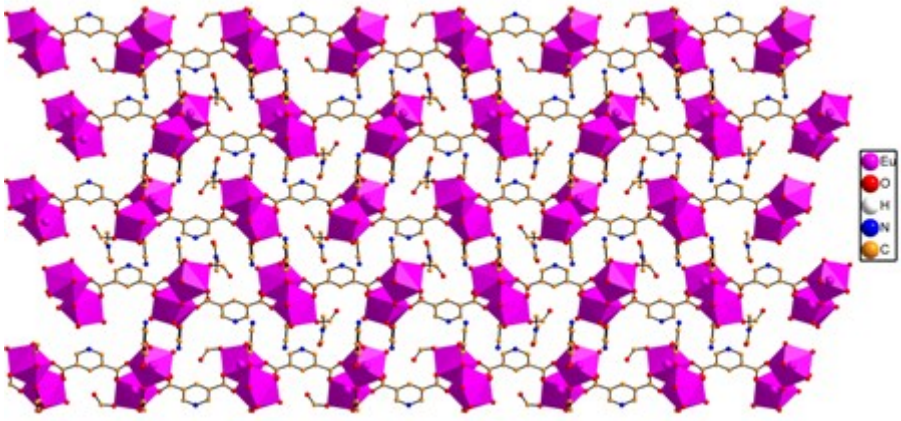

Fig. S4(c) Packing of CP **4** along a-axis.

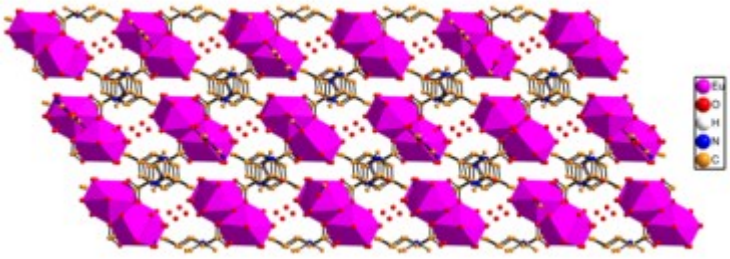

Fig. S4(d) Rhombohedral view of CP **4** along b-axis.

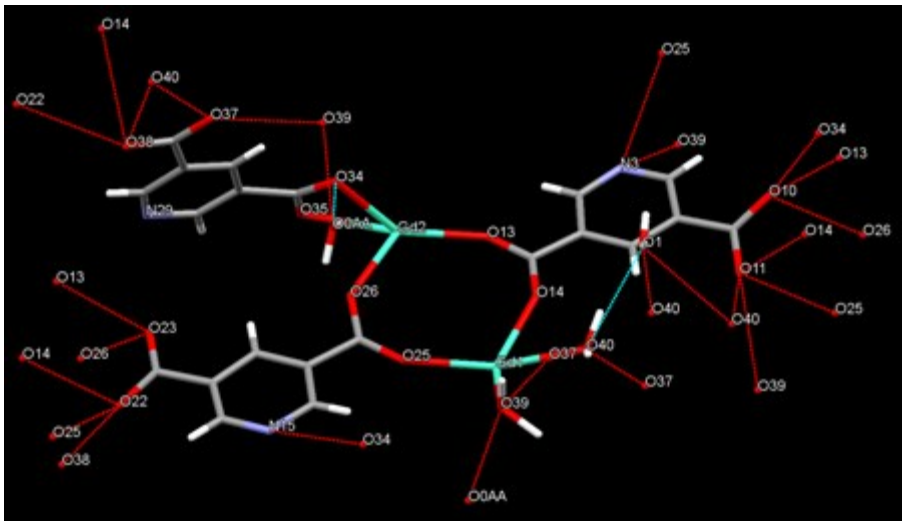

Fig. S5(a) Number and positions of Hydrogen bonds in asymmetric unit of CP **5**.

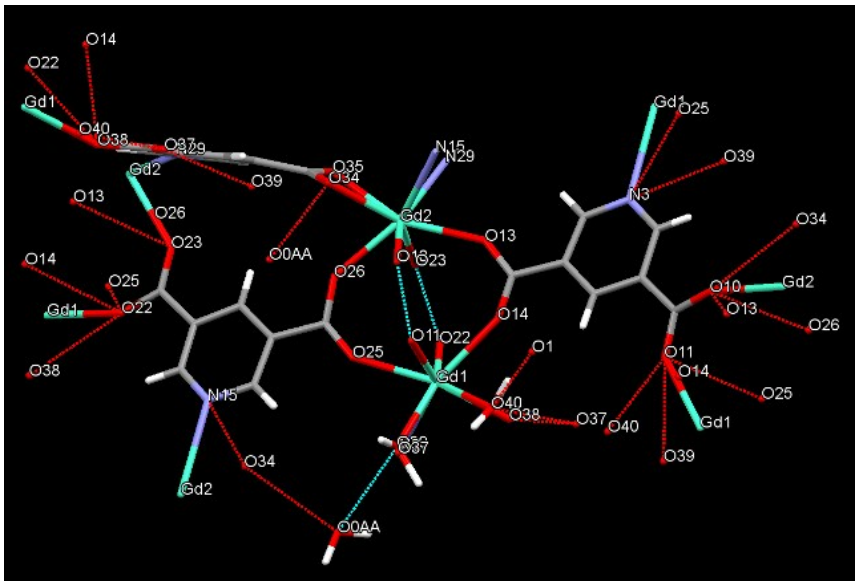

Fig. S5(b) Number and positions of Hydrogen bonds in CP **5**.

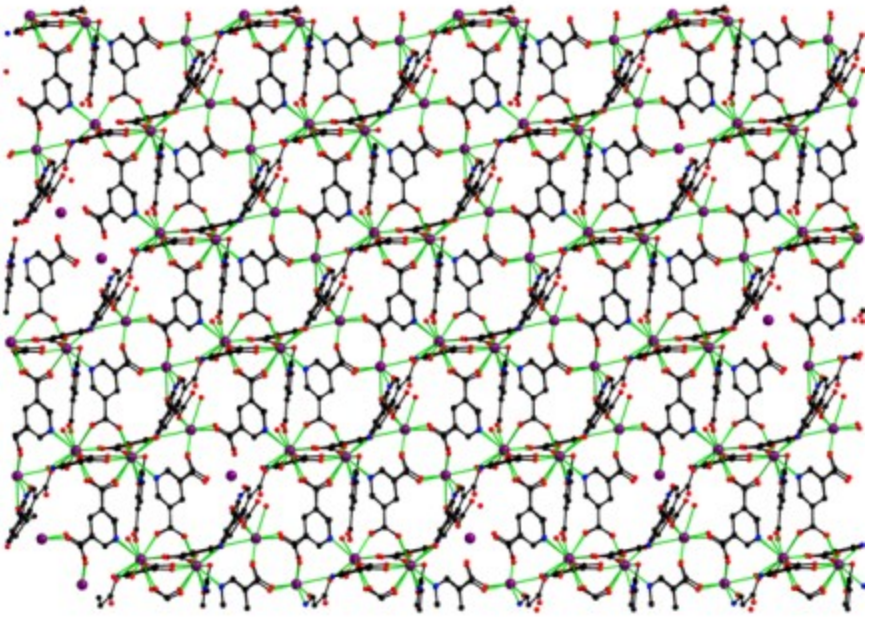

Fig.S5(c) Packing of CP **5** along a-axis.

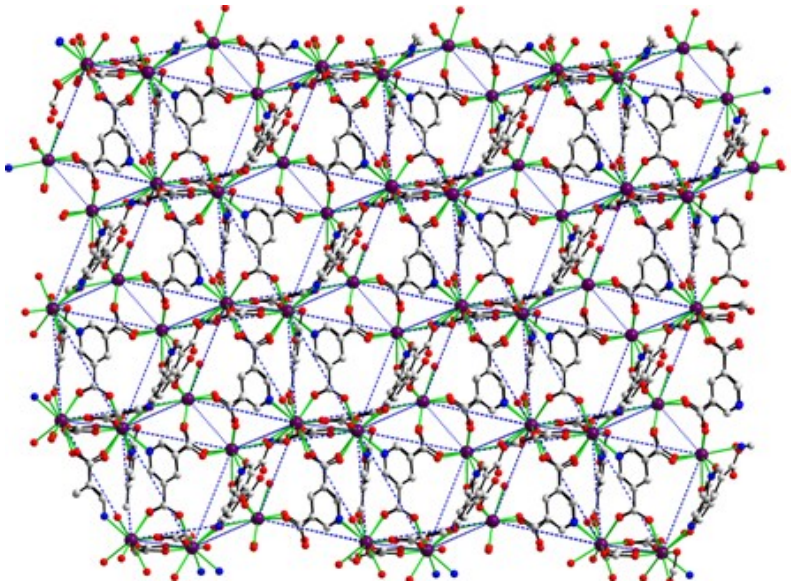

Fig. S5(d) Topology of CP **5** by joining metal centre (dotted blue lines).

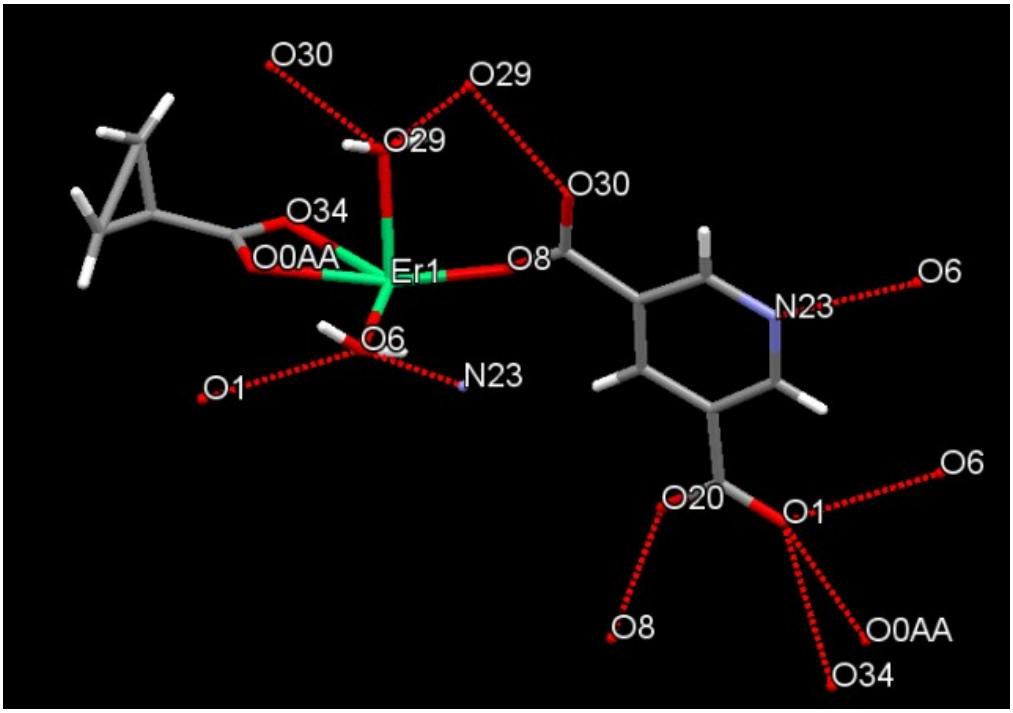

Fig. S6(a) Number and positions of Hydrogen bonds in asymmetric unit of CP **6**.

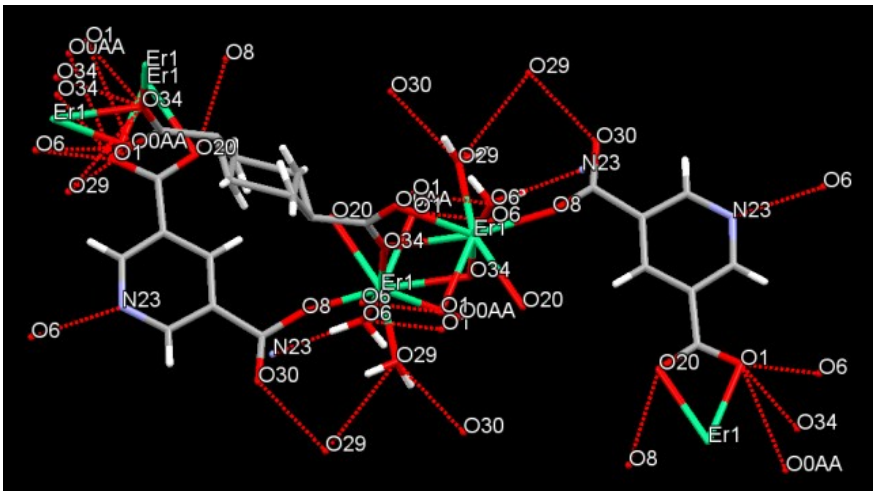

Fig. S6(b) Number and positions of Hydrogen bonds in CP **6**.

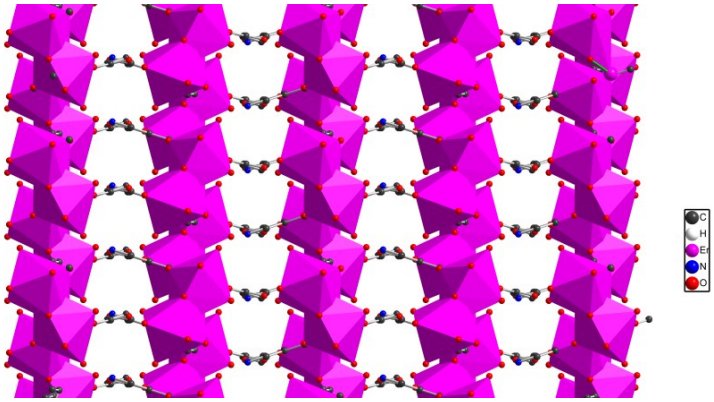

Fig. S6(c) Packing of CP **6** along a-axis.

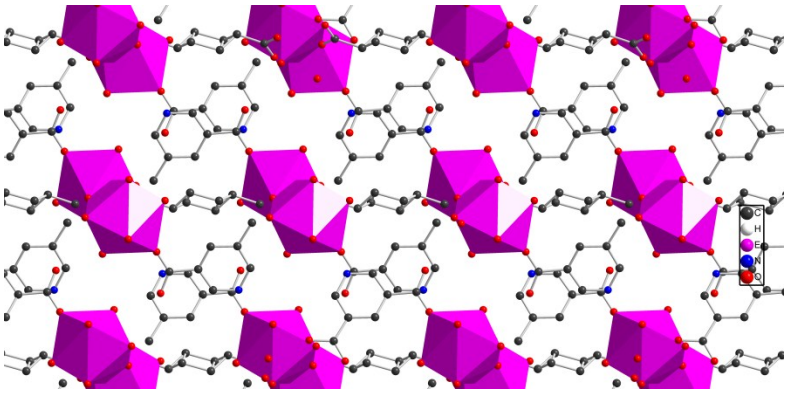

Fig. S6(d) Packing of CP **6** along c-axis.

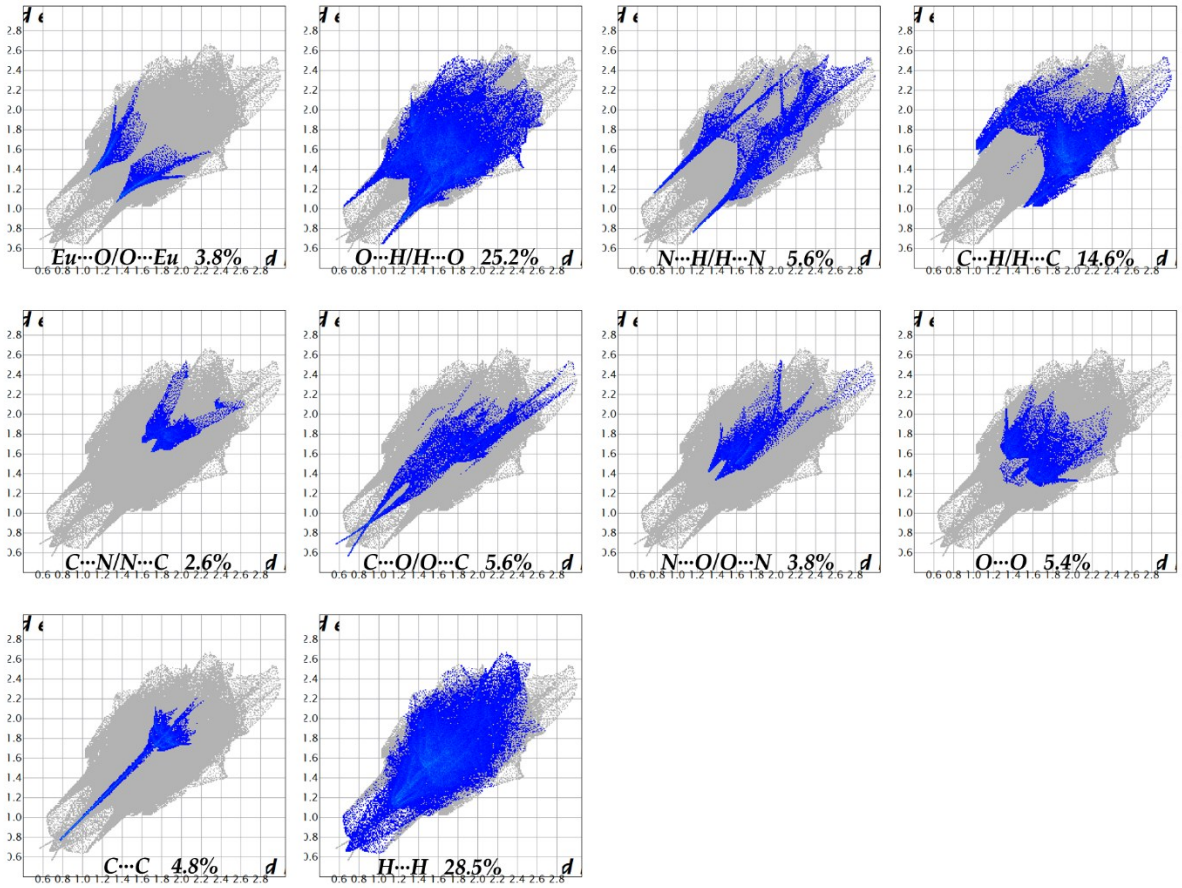

Fig. S7 Full fingerprint plot is resolved into various contacts and showing the percentages of contacts contributed to the total Hirshfeld surface area of molecules of Eu complex.

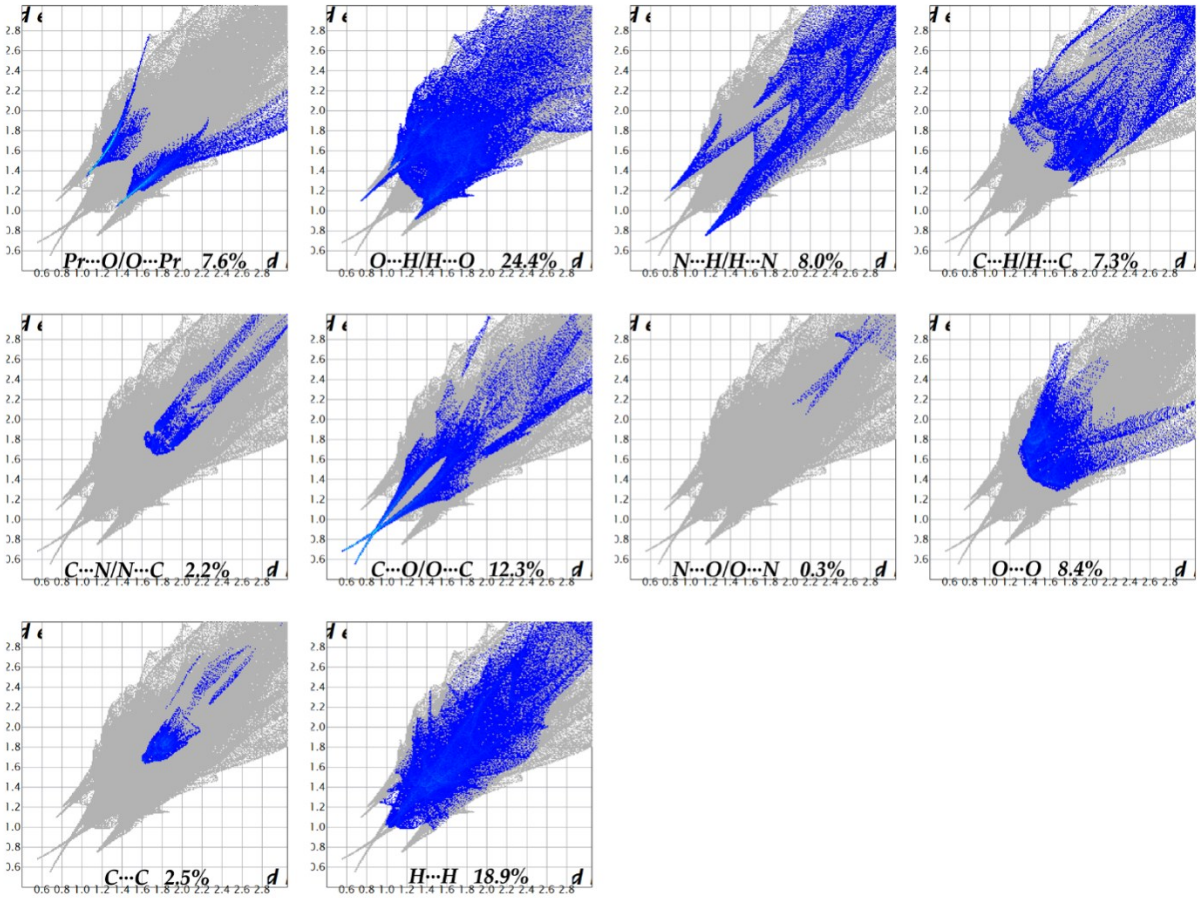

Fig. S8 Full fingerprint plot is resolved into various contacts and showing the percentages of contacts contributed to the total Hirshfeld surface area of molecules of Pr complex.

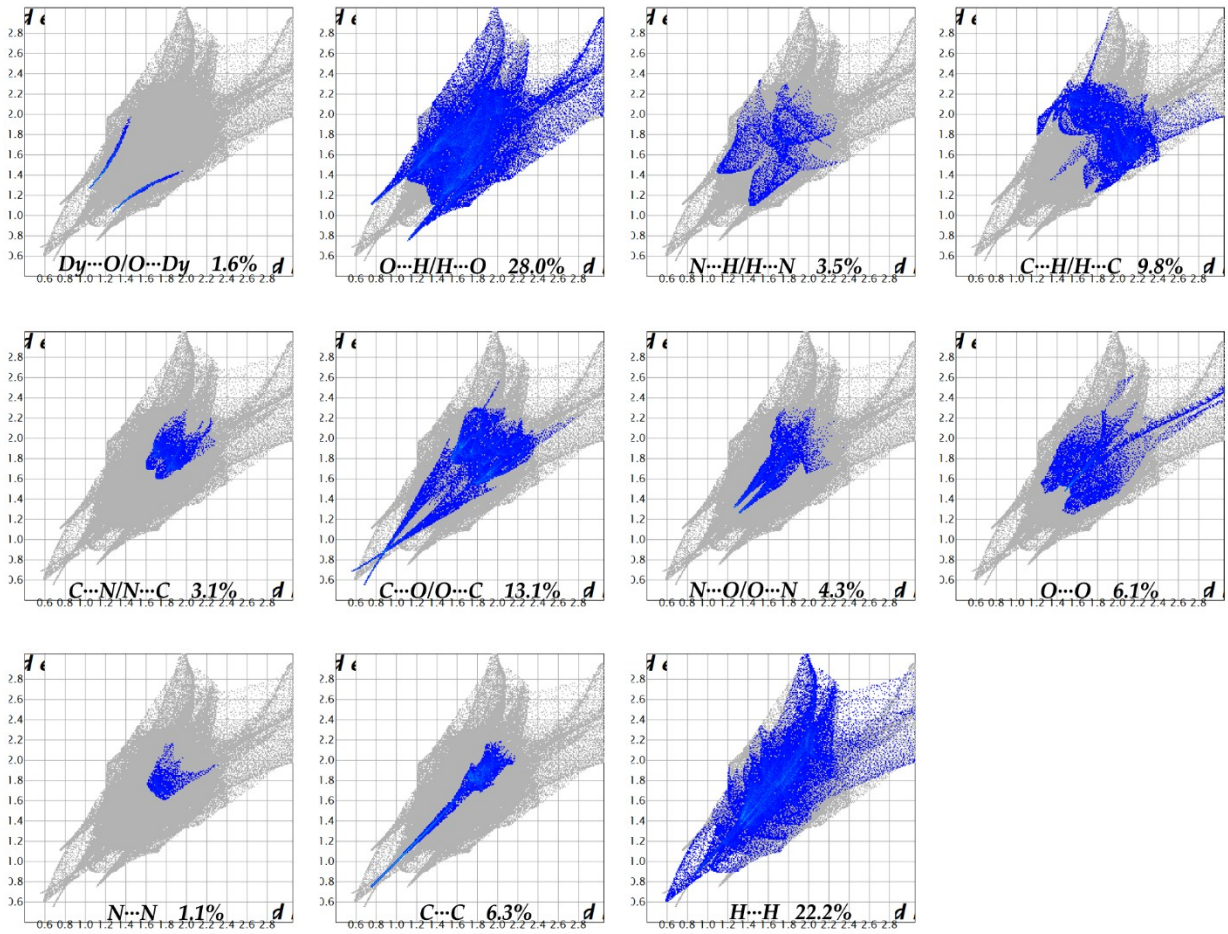

Fig. S9 Full fingerprint plot is resolved into various contacts and showing the percentages of contacts contributed to the total Hirshfeld surface area of molecules of Dy complex.

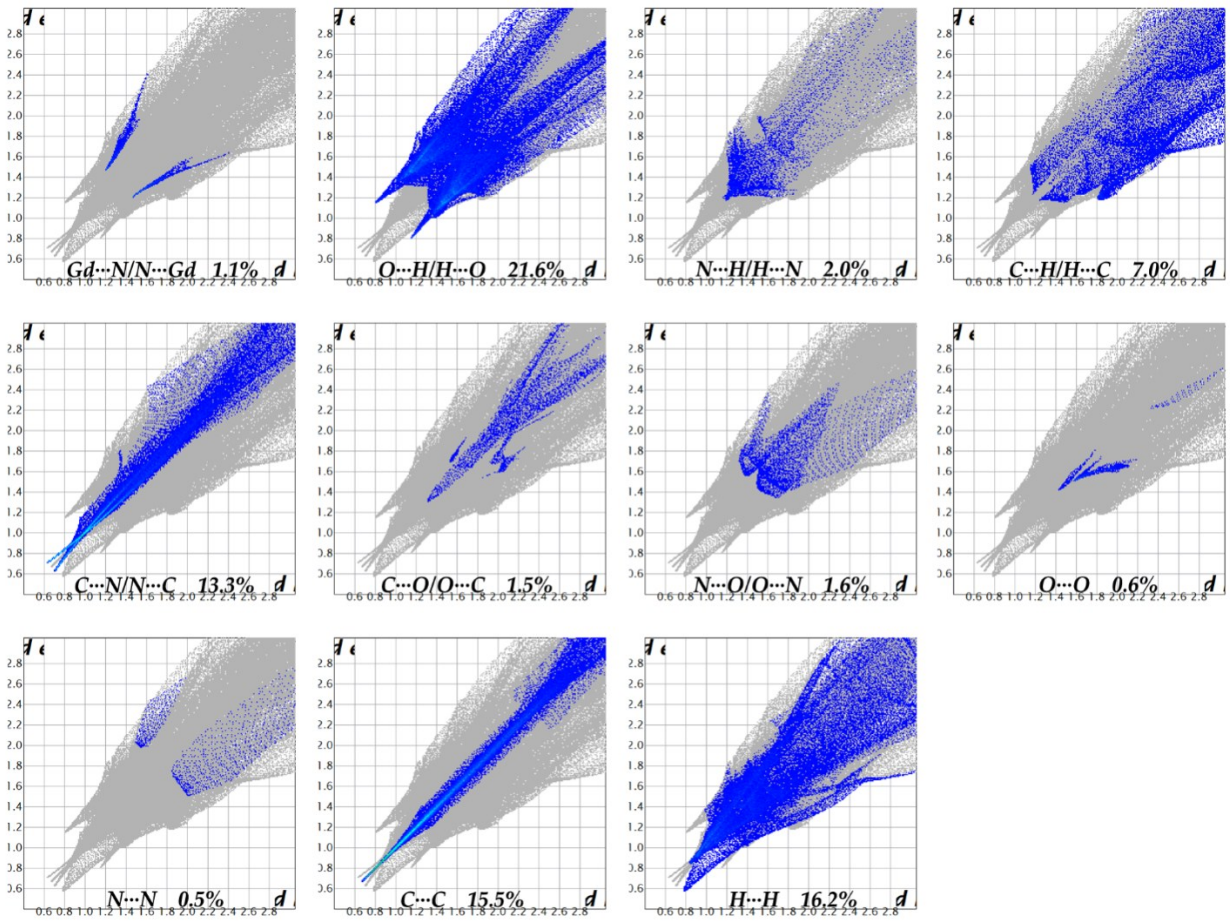

Fig. S10 Full fingerprint plot is resolved into various contacts and showing the percentages of contacts contributed to the total Hirshfeld surface area of molecules of Gd complex.

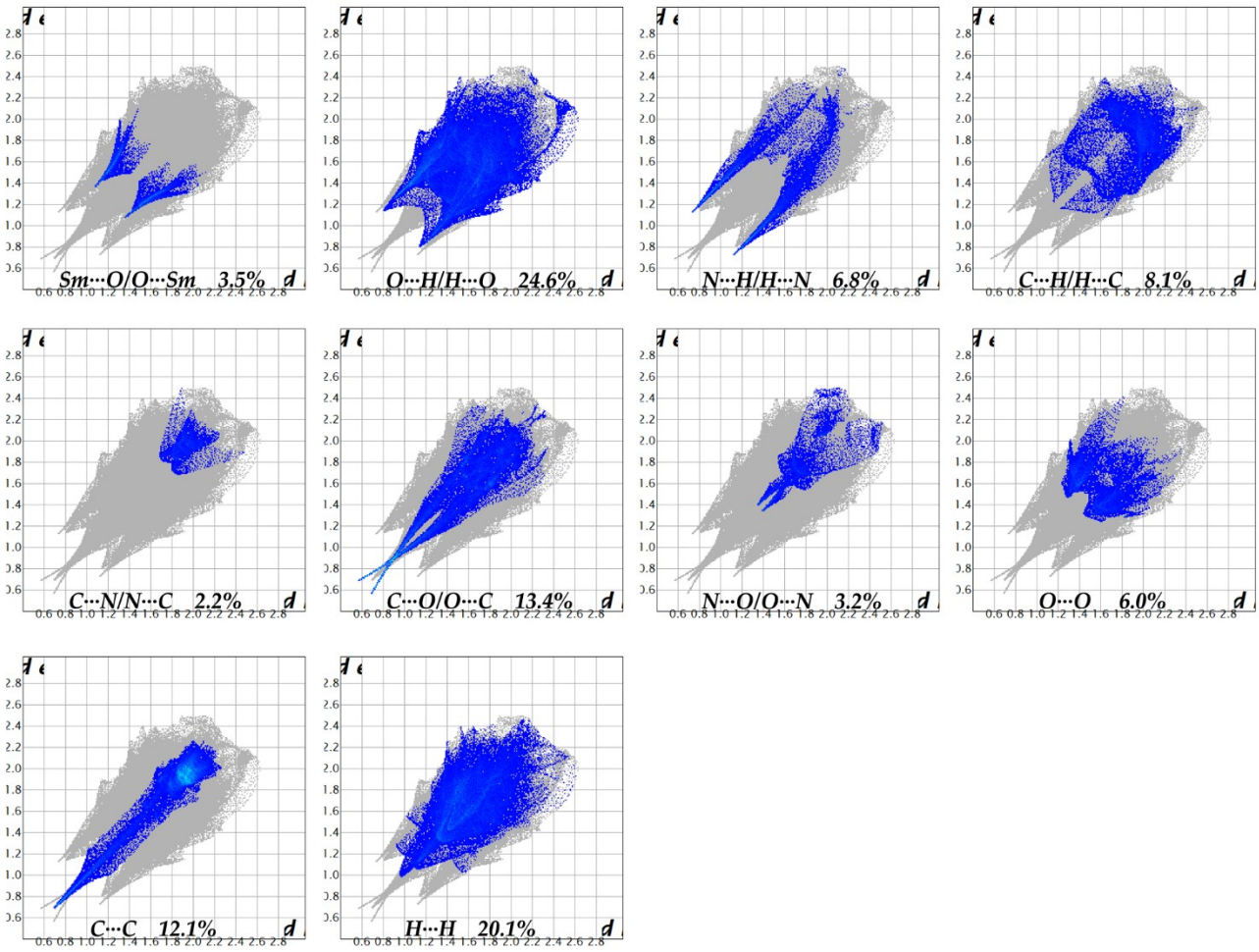

Fig. S11 Full fingerprint plot is resolved into various contacts and showing the percentages of contacts contributed to the total Hirshfeld surface area of molecules of Sm complex.

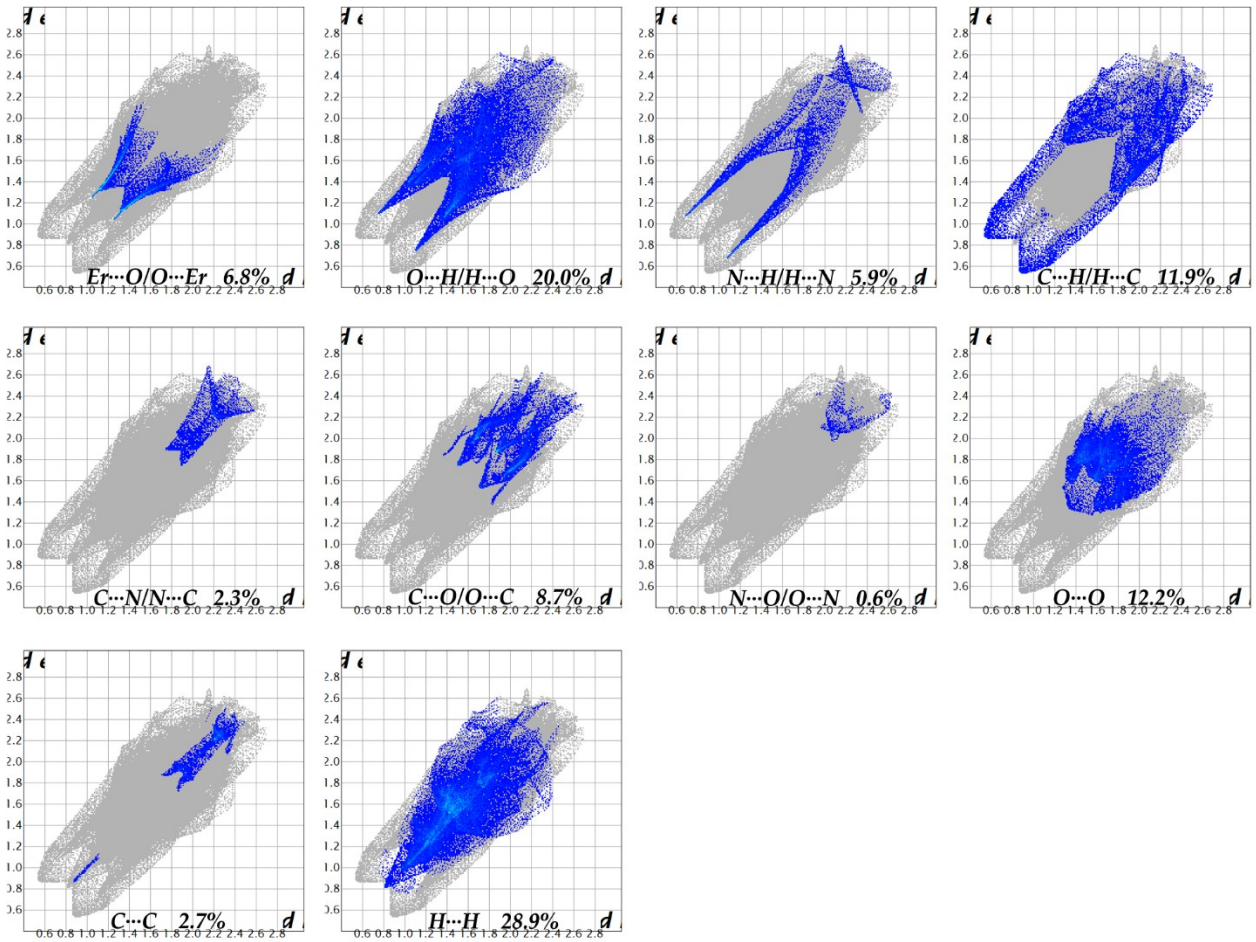

Fig. S12 Full fingerprint plot is resolved into various contacts and showing the percentages of contacts contributed to the total Hirshfeld surface area of molecules of Er complex.

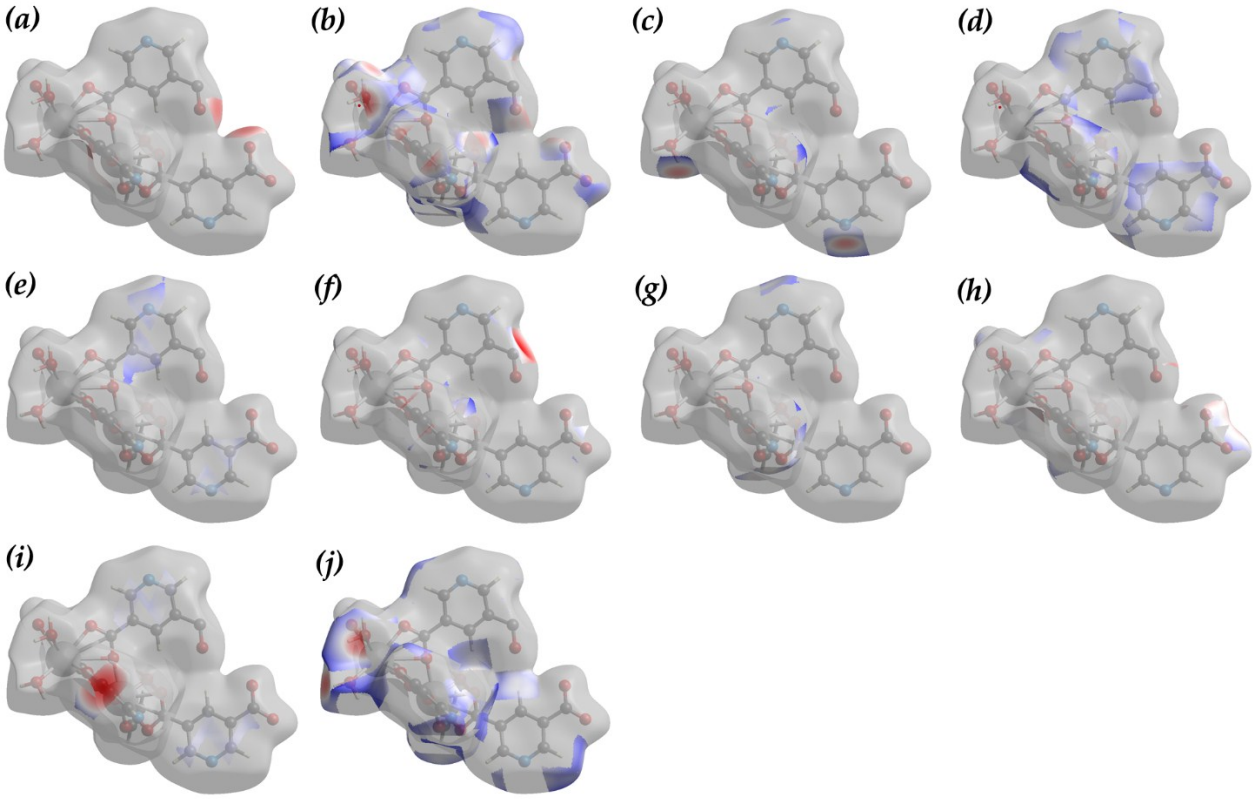

Fig. S13 Hirshfeld surface (d_{norm}) is resolved into Eu···O/O···Eu; O···H/H···O; N···H/H···N; C···H/H···C; C···N/N···C; C···O/O···C; N···O/O···N; O···O; C···C and H···H contacts (a-j) for Eu complex.

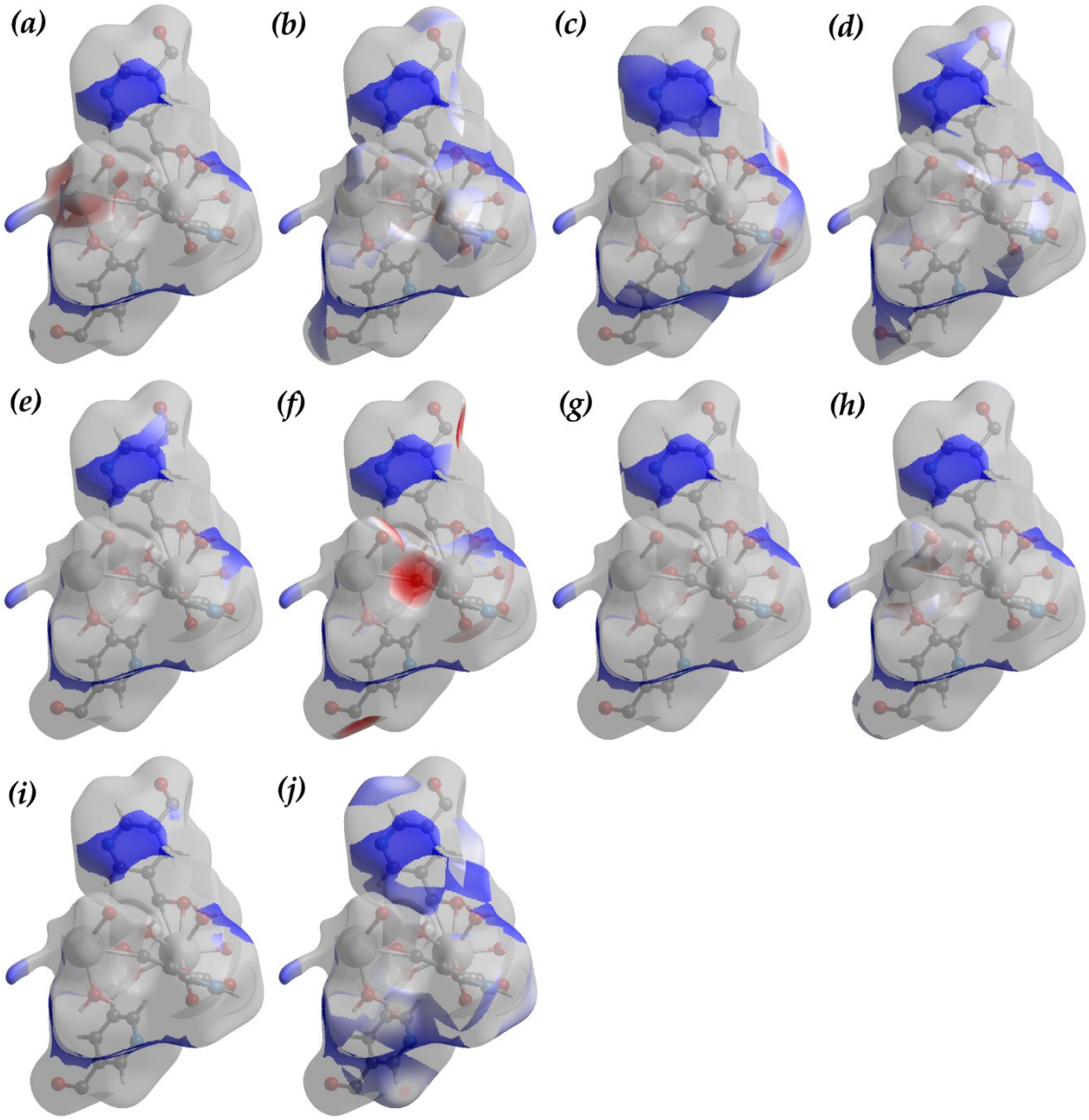

Fig. S14 Hirshfeld surface (d_{norm}) is resolved into Eu···O/O···Eu; O···H/H···O; N···H/H···N; C···H/H···C; C···N/N···C; C···O/O···C; N···O/O···N; O···O; C···C and H···H contacts (a-j) for Pr complex.

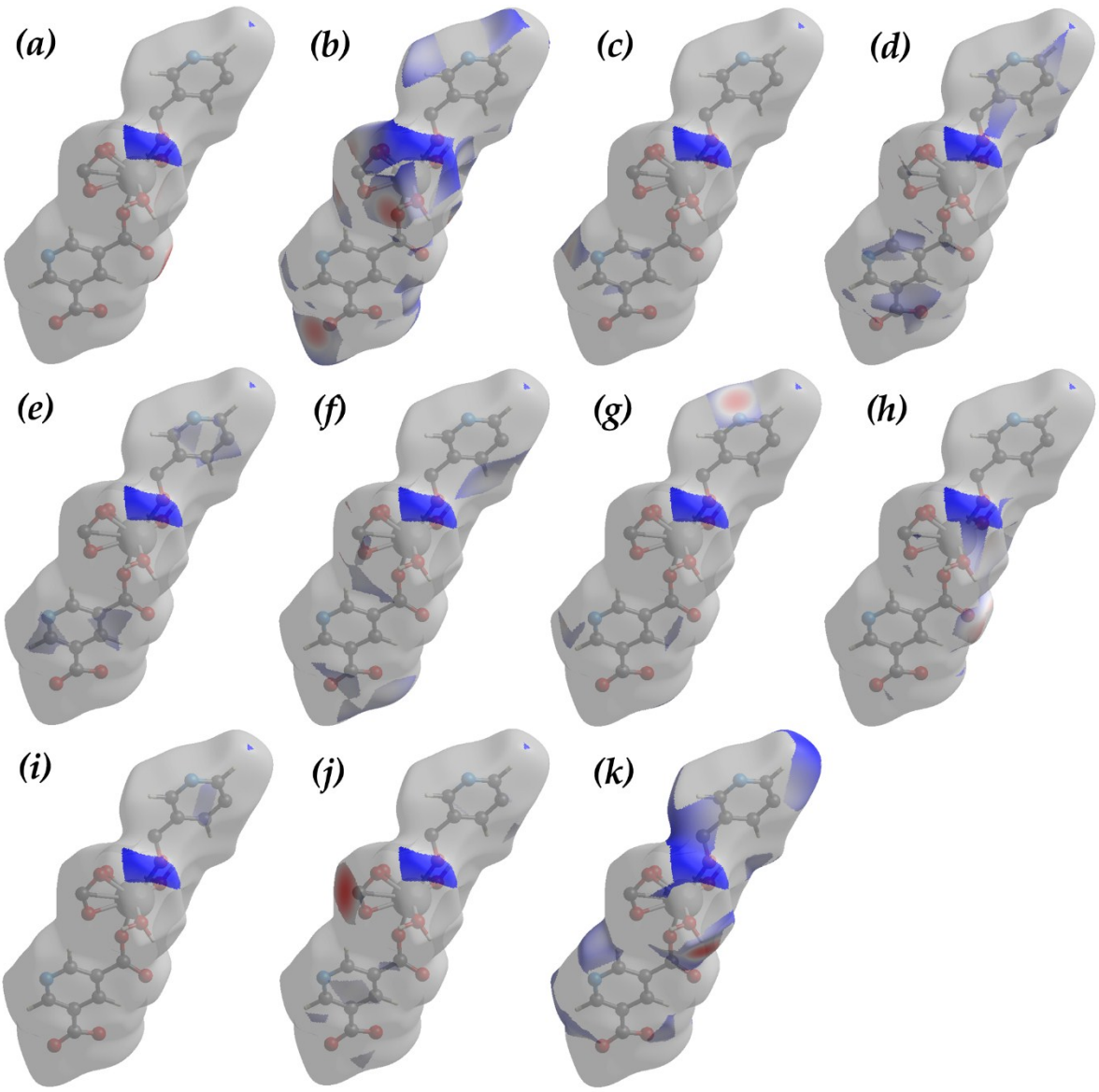

Fig. S15 Hirshfeld surface (d_{norm}) is resolved into Eu···O/O···Eu; O···H/H···O; N···H/H···N; C···H/H···C; C···N/N···C; C···O/O···C; N···O/O···N; O···O; O···O; C···C and H···H contacts (a-k) for Dy complex.

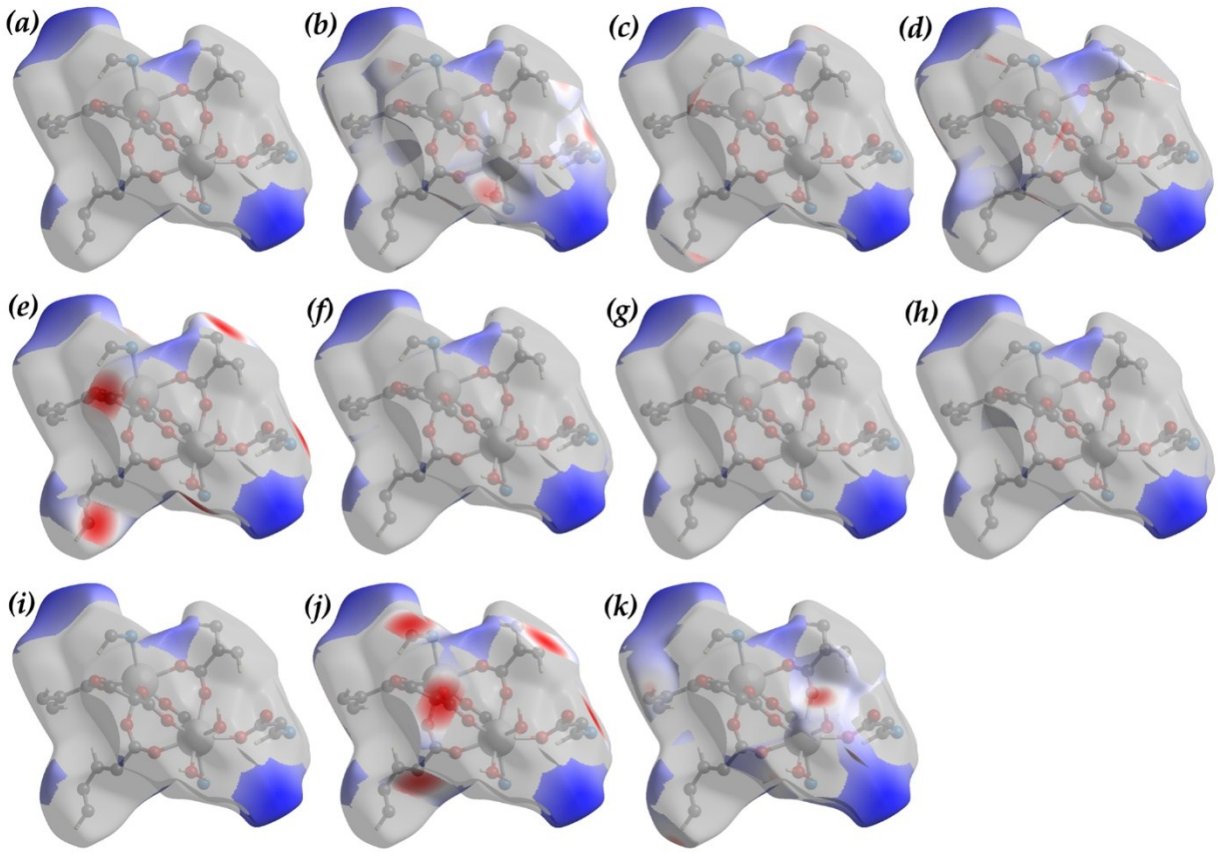

Fig. S16 Hirshfeld surface (d_{norm}) is resolved into Eu···O/O···Eu; O···H/H···O; N···H/H···N; C···H/H···C; C···N/N···C; C···O/O···C; N···O/O···N; O···O; O···O; C···C and H···H contacts (a-k) for Gd complex.

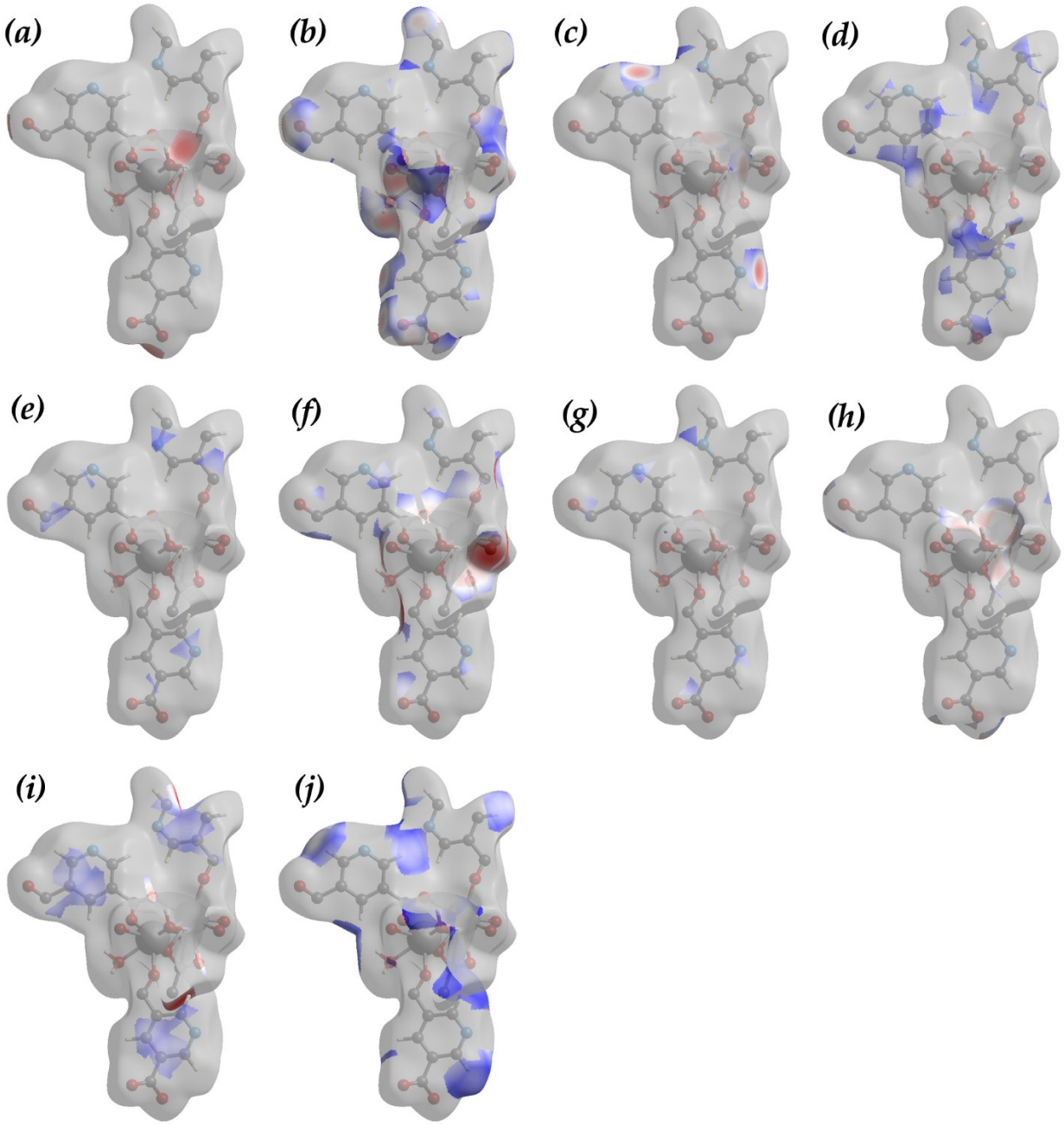

Fig. S17 Hirshfeld surface (d_{norm}) is resolved into Eu···O/O···Eu; O···H/H···O; N···H/H···N; C···H/H···C; C···N/N···C; C···O/O···C; N···O/O···N; O···O; C···C and H···H contacts (a-j) for Sm complex.

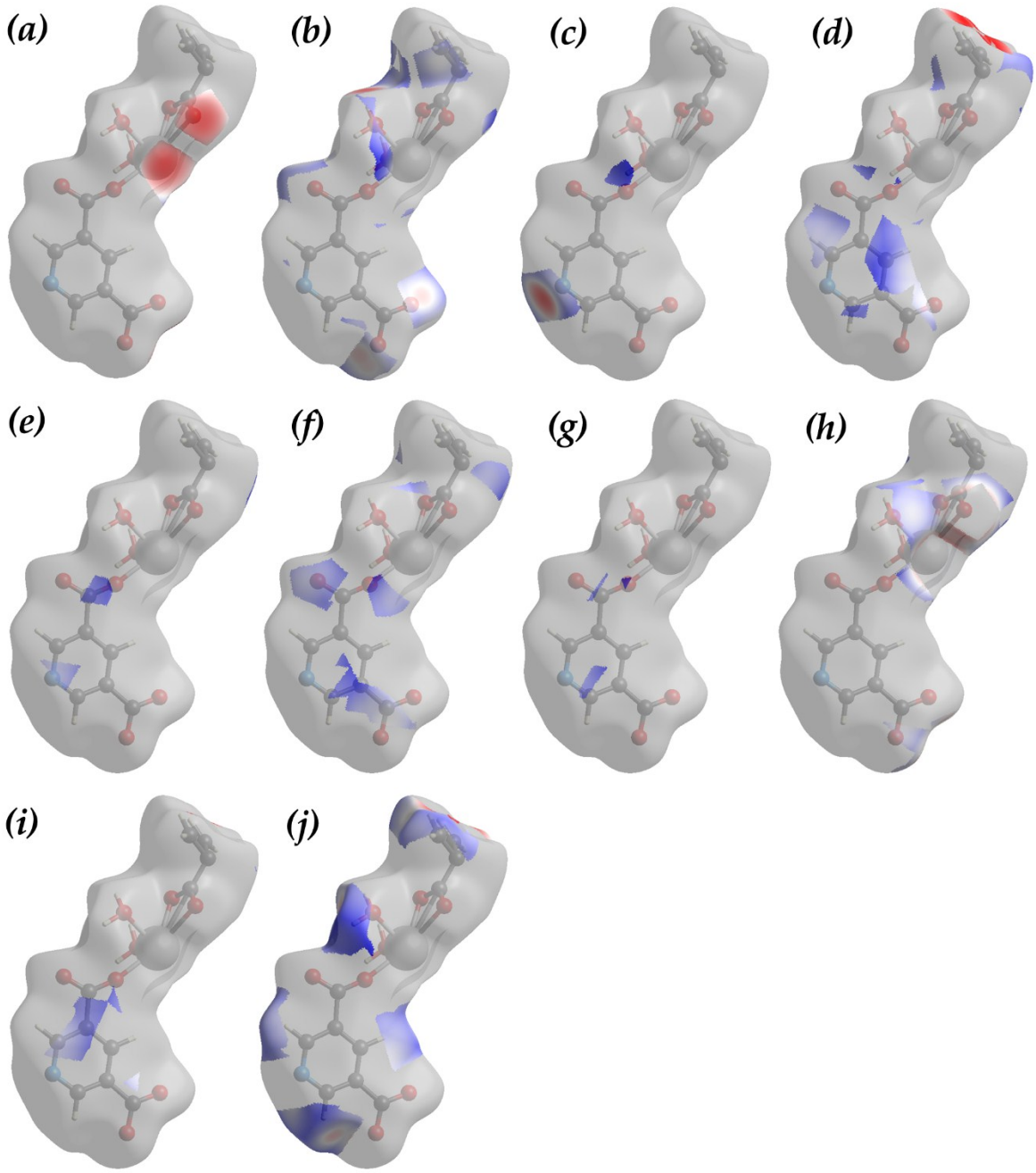

Fig. S18 Hirshfeld surface (d_{norm}) is resolved into Eu···O/O···Eu; O···H/H···O; N···H/H···N; C···H/H···C; C···N/N···C; C···O/O···C; N···O/O···N; O···O; C···C and H···H contacts (a-j) for Er complex.

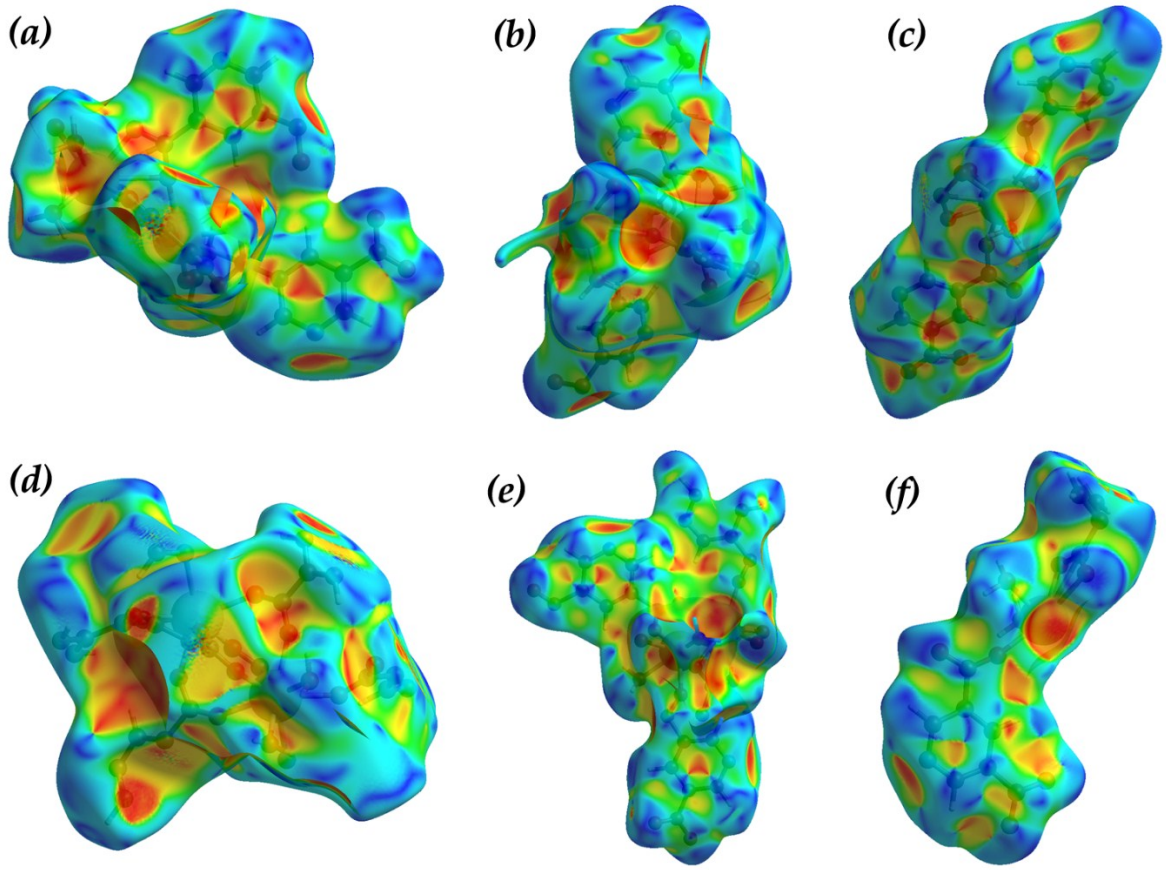

Fig. S19 Shape-index surfaces mapped in the range (-1.000 to 1.000Å) for Eu, Pr, Dy, Gd, Sm and Er complexes (a-f).

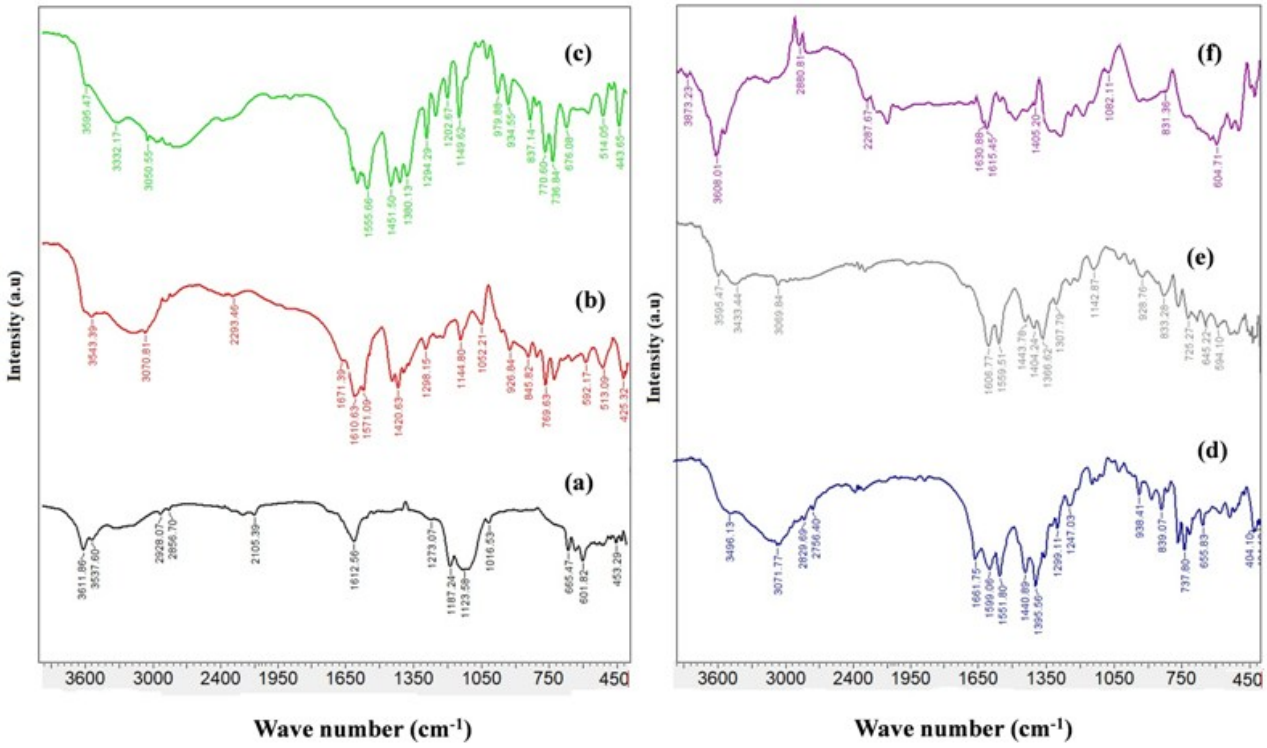

Fig. S20 FT-IR Spectra of CP **1-6.**

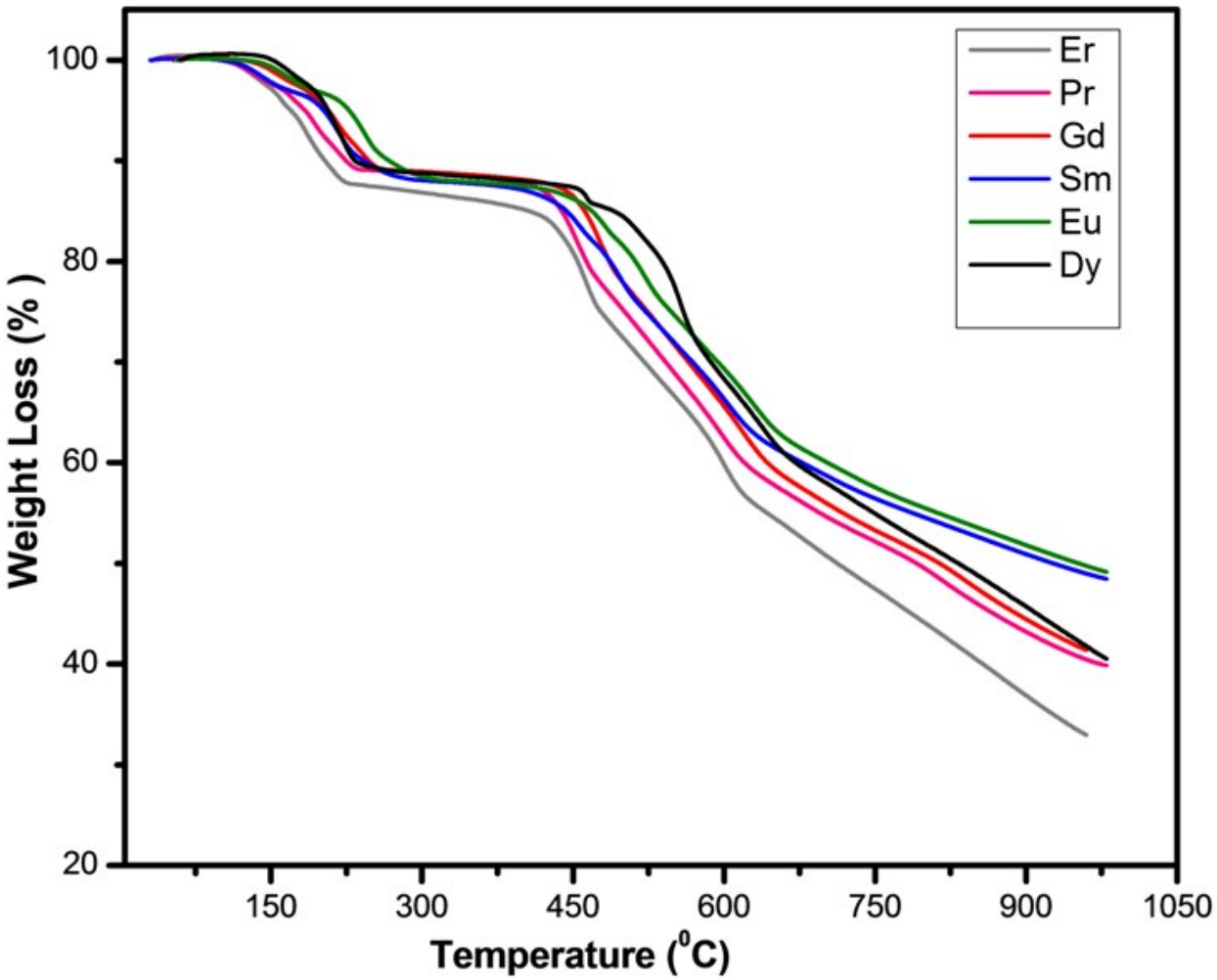

Fig. S21 TGA plots of CP **1-6.**

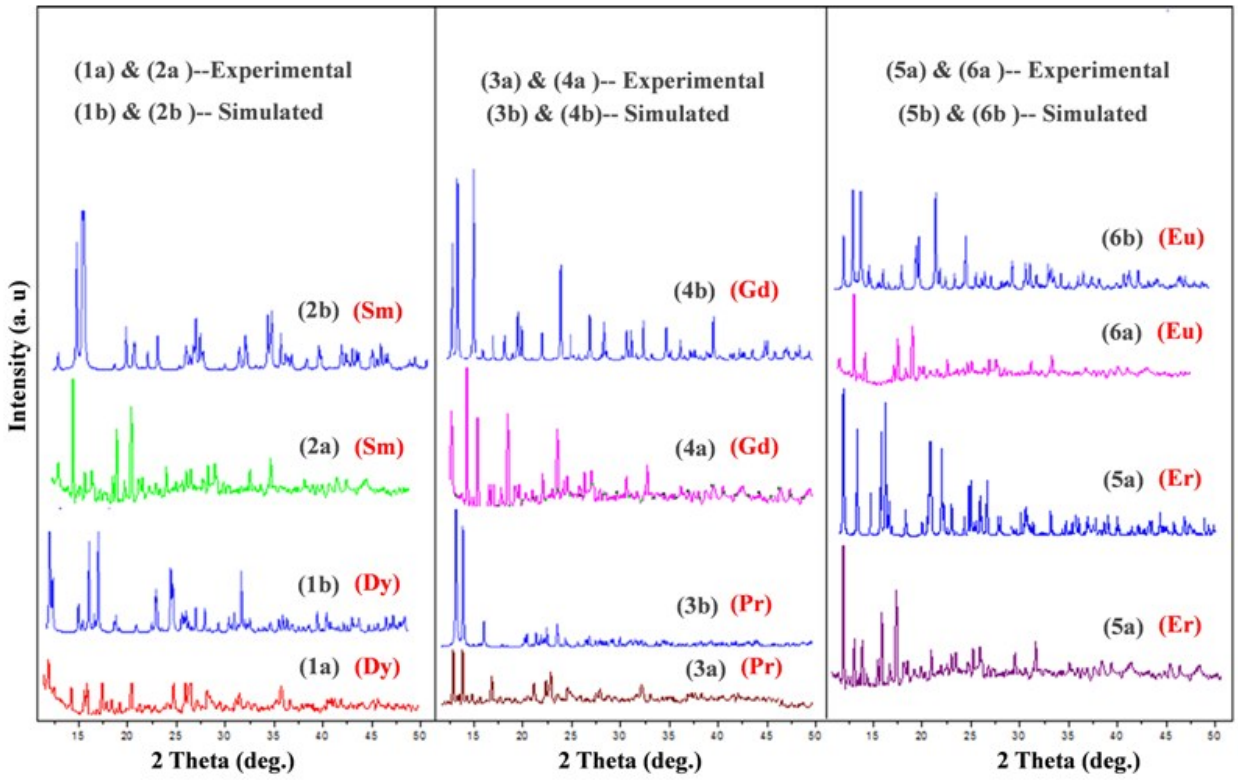

Fig. S22 Experimental and simulated powder X-ray diffraction pattern for CPs **1–6.**

Table S 1. Bond lengths [Å] and angles [°] for CP **1-6**.

Selected Bond lengths CP1
Table S1

C3—C23 1.487(14)	Dy1—O6 2.646(9)
C3—O17^{2_665} 1.237(12)	Dy1—O7 2.407(8)
C8—C10 1.377(15)	Dy1—O9^{2_666} 2.283(8)
C8—C11 1.513(13)	Dy1—O12 2.261(8)
C8—C25 1.376(16)	Dy1—O17 2.284(7)
C14—C23 1.374(14)	N2—C15 1.329(14)
C14—C28 1.381(15)	N2—C19 1.336(14)
C15—C28 1.382(15)	N5—C10 1.323(14)
C17—C28^{1_455}1.491(15)	N5—C31 1.345(16)
C19—C23 1.410(15)	O0AA—C29 1.194(13)
C22—C25 1.383(15)	O2—C3 1.255(13)
C22—C29 1.516(14)	O6—C17 1.265(15)
C22—C31 1.384(16)	O7—C17 1.238(16)
C28—C17^{1_655} 1.491(15)	O9—C11 1.241(12)
Dy1—C17 2.888(11)	O9—Dy1^{2_666} 2.283(8)
Dy1—O2 2.328(8)	O12—C11 1.261(13)
Dy1—O3 2.452(7)	O17—C3^{2_665} 1.237(12)
Dy1—O4 2.353(7)	O19—C29 1.287(13)

Selected Bond angles CP1
Table S2

O2—C3—C23 117.2(9)	O3—Dy1—O6 135.0(3)
O17^{2_665}—C3—C23 117.2(9)	O4—Dy1—C17 73.1(3)
O17^{2_665}—C3—O2 125.6(9)	O4—Dy1—O3 142.2(3)
C10—C8—C11 121.1(9)	O4—Dy1—O6 73.9(3)
C25—C8—C10 119.4(9)	O4—Dy1—O7 73.9(3)
C25—C8—C11 119.6(9)	O6—Dy1—C17 26.0(3)
N5—C10—C8 123.6(9)	O7—Dy1—C17 25.0(3)
O9—C11—C8 117.6(9)	O7—Dy1—O3 140.8(3)
O9—C11—O12 124.3(9)	O7—Dy1—O6 50.9(3)
O12—C11—C8 118.0(8)	O9^{2_666}—Dy1—C17 144.3(3)
C23—C14—C28 120.5(10)	O9^{2_666}—Dy1—O2 80.6(3)
N2—C15—C28 122.4(9)	O9^{2_666}—Dy1—O3 71.4(3)
C28^{1_455}—C17—Dy1 172.3(8)	O9^{2_666}—Dy1—O4 71.4(3)
O6—C17—C28^{1_455} 119.7(11)	O9^{2_666}—Dy1—O6 138.0(3)

O6—C17—Dy1	66.3(6)
O7—C17—C28^{1_455}	118.9(11)
O7—C17—Dy1	55.2(6)
O7—C17—O6	121.4(10)
N2—C19—C23	121.2(9)
C25—C22—C29	121.1(9)
C25—C22—C31	118.8(10)
C31—C22—C29	120.1(9)
C14—C23—C3	120.9(9)
C14—C23—C19	117.8(10)
C19—C23—C3	121.3(9)
C8—C25—C22	118.1(10)
C14—C28—C17^{1_655}	118.7(10)
C15—C28—C14	118.0(9)
C15—C28—C17^{1_655}	123.3(10)
O0AA—C29—C22	122.2(10)
O0AA—C29—O19	125.4(10)
O19—C29—C22	112.3(9)
N5—C31—C22	123.0(10)
O2—Dy1—C17	102.0(3)
O2—Dy1—O3	78.8(3)
O2—Dy1—O4	89.0(3)
O2—Dy1—O6	76.0(3)
O2—Dy1—O7	126.7(3)
O3—Dy1—C17	144.3(3)
O9^{2_666}—Dy1—O7	134.9(3)
O9^{2_666}—Dy1—O17	139.7(3)
O12—Dy1—C17	97.0(3)
O12—Dy1—O2	161.0(4)
O12—Dy1—O3	84.8(3)
O12—Dy1—O4	98.2(3)
O12—Dy1—O6	122.9(3)
O12—Dy1—O7	72.2(3)
O12—Dy1—O9^{2_666}	85.1(3)
O12—Dy1—O17	87.1(3)
O17—Dy1—C17	75.9(3)
O17—Dy1—O2	95.8(3)
O17—Dy1—O3	68.5(3)
O17—Dy1—O4	149.0(3)
O17—Dy1—O6	77.6(3)
O17—Dy1—O7	78.8(3)
C15—N2—C19	120.0(9)
C10—N5—C31	117.1(9)
C3—O2—Dy1	131.4(7)
C17—O6—Dy1	87.7(7)
C17—O7—Dy1	99.8(7)
C11—O9—Dy1^{2_666}	172.6(7)
C11—O12—Dy1	154.6(7)
C3^{2_665}—O17—Dy1	150.7(7)

Selected Bond lengths of CP2

Table S3

C0AA—C1AA 1.403(12)	O9—Pr1^{1_545} 2.793(7)
C0AA—C22 1.511(11)	O13—C31 1.245(10)
C0AA—C33 1.369(12)	O13—Pr1^{2_576} 2.404(6)
C1AA—N8 1.329(12)	O16—C30^{2_667} 1.234(10)
C2AA—C18 1.390(12)	O17—C37 1.228(11)
C3AA—C14 1.508(11)	O17—Pr1^{1_545} 2.565(6)
C3AA—C15 1.400(12)	O20—C22 1.249(11)
C3AA—C33 1.381(12)	O20—Pr1^{1_645} 2.393(6)
C5—C20 1.364(13)	O21—C14 1.263(11)
C9—C27 1.502(11)	O24—C9 1.238(11)

C9—O25^{1_545} 1.264(10)	O25—C9^{1_565} 1.264(10)
C14—O9^{1_565} 1.250(10)	O25—Pr2^{1_565} 2.756(6)
C18—C30 1.510(11)	Pr1—C14 3.060(8)
C18—C42 1.379(12)	Pr1—C37^{1_565} 2.977(9)
C20—C37 1.503(12)	Pr1—O2^{1_565} 2.686(7)
C20—C42 1.404(12)	Pr1—O6^{2_577} 2.363(6)
C24—C27 1.390(11)	Pr1—O9^{1_565} 2.793(7)
C24—C36 1.380(11)	Pr1—O13^{2_576} 2.404(6)
C26—C27 1.383(12)	Pr1—O17^{1_565} 2.565(6)
C30—O16^{2_667} 1.234(10)	Pr1—O20^{1_465} 2.393(6)
C31—C36 1.506(11)	Pr1—O21 2.595(7)
C31—O0AA^{2_666} 1.255(10)	Pr1—O25 2.479(6)
C36—C39 1.383(12)	Pr1—O30 2.474(7)
C37—Pr1^{1_545} 2.977(9)	Pr1—Pr2^{1_565} 4.0954(7)
N3—C26 1.329(11)	Pr2—C9 3.065(8)
N3—C39 1.335(11)	Pr2—O0AA 2.353(6)
N8—C15 1.326(12)	Pr2—O2 2.507(6)
N32—C2AA 1.329(12)	Pr2—O3 2.509(7)
N32—C5 1.335(12)	Pr2—O8 2.445(6)
O0AA—C31^{2_666} 1.255(10)	Pr2—O9 2.497(6)
O2—C37 1.273(10)	Pr2—O16 2.408(6)
O2—Pr1^{1_545} 2.686(7)	Pr2—O24 2.646(7)
O6—C30 1.246(11)	Pr2—O25^{1_545} 2.756(6)
O6—Pr1^{2_577} 2.363(6)	Pr2—O28 2.548(7)
O8—C22 1.251(11)	Pr2—Pr1^{1_545} 4.0954(7)
O9—C14^{1_545} 1.249(10)	

Selected Bond angles of CP2

Table S4

C1AA—C0AA—C22 119.5(8)	O13^{2_576}—Pr1—O2^{1_565} 147.8(2)
C33—C0AA—C1AA 117.7(8)	O13^{2_576}—Pr1—O9^{1_565} 101.3(2)
C33—C0AA—C22 122.8(8)	O13^{2_576}—Pr1—O17^{1_565} 151.8(2)
N8—C1AA—C0AA 123.8(8)	O13^{2_576}—Pr1—O21 68.7(2)
N32—C2AA—C18 123.8(8)	O13^{2_576}—Pr1—O25 81.8(2)
C15—C3AA—C14 118.5(8)	O13^{2_576}—Pr1—O30 125.4(3)
C33—C3AA—C14 123.1(8)	O13^{2_576}—Pr1—Pr2^{1_565} 115.00(16)
C33—C3AA—C15 118.4(8)	O17^{1_565}—Pr1—C14 121.2(2)
N32—C5—C20 123.8(9)	O17^{1_565}—Pr1—C37^{1_565} 24.2(2)
C27—C9—Pr2 170.7(6)	O17^{1_565}—Pr1—O2^{1_565} 49.02(19)

O24—C9—C27	120.3(8)
O24—C9—O25^{1_545}	122.2(8)
O24—C9—Pr2	58.8(5)
O25^{1_545}—C9—C27	117.5(8)
O25^{1_545}—C9—Pr2	64.0(5)
C3AA—C14—Pr1	166.1(6)
O9^{1_565}—C14—C3AA	120.0(8)
O9^{1_565}—C14—O21	121.6(8)
O9^{1_565}—C14—Pr1	65.9(5)
O21—C14—C3AA	118.3(8)
O21—C14—Pr1	56.8(4)
N8—C15—C3AA	123.1(8)
C2AA—C18—C30	120.0(7)
C42—C18—C2AA	118.8(8)
C42—C18—C30	121.1(8)
C5—C20—C37	122.4(8)
C5—C20—C42	119.4(8)
C42—C20—C37	118.1(8)
O8—C22—C0AA	117.0(8)
O20—C22—C0AA	117.0(8)
O20—C22—O8	126.0(8)
C36—C24—C27	118.2(8)
N3—C26—C27	123.9(8)
C24—C27—C9	121.8(8)
C26—C27—C9	119.6(7)
C26—C27—C24	118.5(8)
O6—C30—C18	116.9(7)
O16^{2_667}—C30—C18	115.9(8)
O16^{2_667}—C30—O6	127.2(8)
O0AA^{2_666}—C31—C36	116.3(7)
O13—C31—C36	117.5(7)
O13—C31—O0AA^{2_666}	126.2(8)
C0AA—C33—C3AA	119.6(8)
C24—C36—C31	120.1(7)
C24—C36—C39	118.7(8)
C39—C36—C31	121.1(7)
C20—C37—Pr1^{1_545}	163.6(6)
O2—C37—C20	117.6(8)
O2—C37—Pr1^{1_545}	64.5(5)
O17—C37—C20	120.9(8)
O17—C37—O2	121.4(8)

O17^{1_565}—Pr1—O9^{1_565}	106.3(2)
O17^{1_565}—Pr1—O21	136.0(2)
O17^{1_565}—Pr1—Pr2^{1_565}	85.45(15)
O20^{1_465}—Pr1—C14	153.7(2)
O20^{1_465}—Pr1—C37^{1_565}	86.3(2)
O20^{1_465}—Pr1—O2^{1_565}	92.3(2)
O20^{1_465}—Pr1—O9^{1_565}	138.4(2)
O20^{1_465}—Pr1—O13^{2_576}	80.7(2)
O20^{1_465}—Pr1—O17^{1_565}	75.2(2)
O20^{1_465}—Pr1—O21	148.7(2)
O20^{1_465}—Pr1—O25	75.9(2)
O20^{1_465}—Pr1—O30	140.6(3)
O20^{1_465}—Pr1—Pr2^{1_565}	104.44(17)
O21—Pr1—C14	24.0(2)
O21—Pr1—C37^{1_565}	123.0(2)
O21—Pr1—O2^{1_565}	110.0(2)
O21—Pr1—O9^{1_565}	47.9(2)
O21—Pr1—Pr2^{1_565}	83.58(16)
O25—Pr1—C14	79.6(2)
O25—Pr1—C37^{1_565}	88.3(2)
O25—Pr1—O2^{1_565}	66.03(19)
O25—Pr1—O9^{1_565}	63.5(2)
O25—Pr1—O17^{1_565}	105.9(2)
O25—Pr1—O21	92.9(2)
O25—Pr1—Pr2^{1_565}	41.00(14)
O30—Pr1—C14	64.7(3)
O30—Pr1—C37^{1_565}	69.3(3)
O30—Pr1—O2^{1_565}	78.8(3)
O30—Pr1—O9^{1_565}	71.0(2)
O30—Pr1—O17^{1_565}	70.0(3)
O30—Pr1—O21	67.7(3)
O30—Pr1—O25	131.1(2)
O30—Pr1—Pr2^{1_565}	90.9(2)
C9—Pr2—Pr1^{1_545}	57.02(16)
O0AA—Pr2—C9	97.9(2)
O0AA—Pr2—O2	150.3(2)
O0AA—Pr2—O3	138.9(3)
O0AA—Pr2—O8	98.6(2)
O0AA—Pr2—O9	84.5(2)
O0AA—Pr2—O16	78.1(2)
O0AA—Pr2—O24	75.6(2)

O17—C37—Pr1^{1_545}	58.8(5)
N3—C39—C36	123.8(8)
C18—C42—C20	117.2(8)
C26—N3—C39	116.8(8)
C15—N8—C1AA	117.5(8)
C2AA—N32—C5	116.8(8)
C31^{2_666}—O0AA—Pr2	156.2(6)
C37—O2—Pr1^{1_545}	90.2(5)
C37—O2—Pr2	163.7(6)
Pr2—O2—Pr1^{1_545}	104.1(2)
C30—O6—Pr1^{2_577}	151.1(6)
C22—O8—Pr2	136.8(6)
C14^{1_545}—O9—Pr1^{1_545}	90.0(5)
C14^{1_545}—O9—Pr2	165.1(6)
Pr2—O9—Pr1^{1_545}	101.3(2)
C31—O13—Pr1^{2_576}	153.6(6)
C30^{2_667}—O16—Pr2	153.8(6)
C37—O17—Pr1^{1_545}	97.1(5)
C22—O20—Pr1^{1_645}	154.6(6)
C14—O21—Pr1	99.1(5)
C9—O24—Pr2	97.6(5)
C9^{1_565}—O25—Pr1	139.4(6)
C9^{1_565}—O25—Pr2^{1_565}	91.7(5)
Pr1—O25—Pr2^{1_565}	102.8(2)
C14—Pr1—Pr2^{1_565}	60.58(17)
C37^{1_565}—Pr1—C14	102.4(2)
C37^{1_565}—Pr1—Pr2^{1_565}	61.59(18)
O2^{1_565}—Pr1—C14	86.2(2)
O2^{1_565}—Pr1—C37^{1_565}	25.3(2)
O2^{1_565}—Pr1—O9^{1_565}	63.83(19)
O2^{1_565}—Pr1—Pr2^{1_565}	36.43(13)
O6^{2_577}—Pr1—C14	120.4(3)
O6^{2_577}—Pr1—C37^{1_565}	101.5(3)
O6^{2_577}—Pr1—O2^{1_565}	126.8(2)
O6^{2_577}—Pr1—O9^{1_565}	140.6(2)
O6^{2_577}—Pr1—O13^{2_576}	83.4(2)
O6^{2_577}—Pr1—O17^{1_565}	78.6(2)
O6^{2_577}—Pr1—O20^{1_465}	81.0(2)
O6^{2_577}—Pr1—O21	101.2(3)
O6^{2_577}—Pr1—O25	154.3(2)
O6^{2_577}—Pr1—O30	74.6(3)
O0AA—Pr2—O25^{1_545}	119.0(2)
O0AA—Pr2—O28	71.5(2)
O0AA—Pr2—Pr1^{1_545}	124.42(18)
O2—Pr2—C9	88.9(2)
O2—Pr2—O3	70.7(2)
O2—Pr2—O24	112.2(2)
O2—Pr2—O25^{1_545}	64.59(19)
O2—Pr2—O28	138.2(2)
O2—Pr2—Pr1^{1_545}	39.51(15)
O3—Pr2—C9	74.4(2)
O3—Pr2—O24	86.8(3)
O3—Pr2—O25^{1_545}	67.3(2)
O3—Pr2—O28	67.6(3)
O3—Pr2—Pr1^{1_545}	85.70(19)
O8—Pr2—C9	143.1(2)
O8—Pr2—O2	92.8(2)
O8—Pr2—O3	71.5(2)
O8—Pr2—O9	144.6(2)
O8—Pr2—O24	139.5(2)
O8—Pr2—O25^{1_545}	137.5(2)
O8—Pr2—O28	71.1(3)
O8—Pr2—Pr1^{1_545}	132.23(16)
O9—Pr2—C9	69.8(2)
O9—Pr2—O2	70.8(2)
O9—Pr2—O3	127.0(2)
O9—Pr2—O24	75.6(2)
O9—Pr2—O25^{1_545}	63.9(2)
O9—Pr2—O28	141.0(3)
O9—Pr2—Pr1^{1_545}	41.97(15)
O16—Pr2—C9	141.9(2)
O16—Pr2—O2	78.9(2)
O16—Pr2—O3	132.2(3)
O16—Pr2—O8	74.1(2)
O16—Pr2—O9	72.0(2)
O16—Pr2—O24	139.7(3)
O16—Pr2—O25^{1_545}	129.5(2)
O16—Pr2—O28	128.9(3)
O16—Pr2—Pr1^{1_545}	93.76(16)
O24—Pr2—C9	23.6(2)
O24—Pr2—O25^{1_545}	47.79(19)
O24—Pr2—Pr1^{1_545}	77.14(16)

O6^{2_577}—Pr1—Pr2^{1_565} 161.30(17)	O25^{1_545}—Pr2—C9 24.3(2)
O9^{1_565}—Pr1—C14 24.1(2)	O25^{1_545}—Pr2—Pr1^{1_545} 36.18(12)
O9^{1_565}—Pr1—C37^{1_565} 83.8(2)	O28—Pr2—C9 83.3(3)
O9^{1_565}—Pr1—Pr2^{1_565} 36.71(13)	O28—Pr2—O24 69.0(3)
O13^{2_576}—Pr1—C14 86.6(2)	O28—Pr2—O25^{1_545} 101.3(2)
O13^{2_576}—Pr1—C37^{1_565} 165.3(2)	O28—Pr2—Pr1^{1_545} 137.3(2)

Selected Bond lengths of CP3
Table S5

C5—C25^{1_545} 1.380(7)	O2—Sm2^{4_565} 2.632(4)
C5—C48^{1_545} 1.413(7)	O3—C70 1.294(6)
C5—C70 1.479(8)	O10—C41 1.296(6)
C9—C13 1.390(7)	O10—Sm1^{1_545} 2.406(4)
C9—C41 1.499(7)	O10—Sm2^{1_545} 2.541(4)
C9—C62 1.378(7)	O11—C37 1.256(6)
C11—C0AA 1.389(7)	O14—C74^{3_666} 1.251(6)
C11—C20 1.384(8)	O16—C66^{3_556} 1.249(7)
C11—C30 1.518(7)	O21—C37 1.258(6)
C13—C35 1.382(7)	O33—C30^{4_666} 1.276(7)
C15—C35 1.386(7)	O42—C70 1.234(6)
C24—C0AA 1.388(7)	O44—C41 1.220(6)
C24—C37 1.505(7)	O44—Sm2^{1_545} 2.655(4)
C24—C57 1.371(8)	Sm1—C70 2.943(6)
C25—C5^{1_565} 1.380(7)	Sm1—O1 2.316(4)
C30—O33^{4_565} 1.276(7)	Sm1—O3 2.503(4)
C35—C66 1.506(7)	Sm1—O10^{1_565} 2.406(4)
C41—Sm2^{1_545} 2.966(5)	Sm1—O14 2.368(4)
C44—C48 1.387(7)	Sm1—O21 2.489(4)
C44—C68 1.388(7)	Sm1—O25 2.400(4)
C44—C74 1.510(7)	Sm1—O33 2.366(4)
C48—C5^{1_565} 1.413(7)	Sm1—O42 2.626(4)
C66—O0AA 1.261(6)	Sm2—C41^{1_565} 2.966(5)
C66—O16^{3_556} 1.248(7)	Sm2—O0AA 2.353(4)
C74—O1 1.253(6)	Sm2—O2^{4_666} 2.632(4)
C74—O14^{3_666} 1.251(6)	Sm2—O3 2.434(4)
N16—C15 1.343(7)	Sm2—O10^{1_565} 2.542(4)

N16—C62 1.338(7)	Sm2—O11 2.341(4)
N18—C20 1.332(7)	Sm2—O16 2.398(4)
N18—C57 1.341(7)	Sm2—O40 2.505(4)
N54—C25 1.349(7)	Sm2—O44^{1_565} 2.655(4)
N54—C68 1.337(7)	Sm2—O48 2.434(4)
O2—C30 1.248(7)	Sm2—Sm1 3.8745(4)

Selected Bond angles of CP3
Table S6

C24—C0AA—C11 119.0(6)	O10^{1_565}—Sm1—O21 71.30(12)
C25^{1_545}—C5—C48^{1_545} 117.9(5)	O10^{1_565}—Sm1—O42 115.13(12)
C25^{1_545}—C5—C70 119.7(5)	O10^{1_565}—Sm1—Sm2 39.72(9)
C48^{1_545}—C5—C70 122.4(5)	O14—Sm1—C70 98.80(14)
C13—C9—C41 120.3(5)	O14—Sm1—O3 124.40(13)
C62—C9—C13 119.4(5)	O14—Sm1—O10^{1_565} 143.23(14)
C62—C9—C41 120.4(5)	O14—Sm1—O21 134.63(13)
C0AA—C11—C30 120.5(5)	O14—Sm1—O25 73.62(14)
C20—C11—C0AA 118.0(5)	O14—Sm1—O42 74.19(13)
C20—C11—C30 121.5(5)	O14—Sm1—Sm2 152.46(9)
C35—C13—C9 118.2(5)	O21—Sm1—C70 105.12(14)
N16—C15—C35 123.0(5)	O21—Sm1—O3 82.64(12)
N18—C20—C11 123.7(5)	O21—Sm1—O42 125.30(12)
C0AA—C24—C37 118.6(5)	O21—Sm1—Sm2 71.42(9)
C57—C24—C0AA 118.4(5)	O25—Sm1—C70 78.31(14)
C57—C24—C37 122.9(5)	O25—Sm1—O3 84.07(14)
N54—C25—C5^{1_565} 124.1(5)	O25—Sm1—O10^{1_565} 142.52(13)
O2—C30—C11 118.5(5)	O25—Sm1—O21 74.29(13)
O2—C30—O33^{4_565} 126.3(5)	O25—Sm1—O42 74.17(13)
O33^{4_565}—C30—C11 115.1(5)	O25—Sm1—Sm2 114.16(10)
C13—C35—C15 118.8(5)	O33—Sm1—C70 75.97(14)

C13—C35—C66 121.8(5)
C15—C35—C66 119.3(5)
O11—C37—C24 114.0(5)
O11—C37—O21 125.5(5)
O21—C37—C24 120.5(5)
C9—C41—Sm2^{1_545} 174.1(4)
O10—C41—C9 117.4(5)
O10—C41—Sm2^{1_545} 58.5(3)
O44—C41—C9 120.8(5)
O44—C41—O10 121.8(5)
O44—C41—Sm2^{1_545} 63.4(3)
C48—C44—C68 119.0(5)
C48—C44—C74 121.5(5)
C68—C44—C74 119.6(5)
C44—C48—C5^{1_565} 118.3(5)
N18—C57—C24 123.7(5)
N16—C62—C9 122.8(5)
O0AA—C66—C35 116.4(5)
O16^{3_556}—C66—C35 118.7(5)
O16^{3_556}—C66—O0AA 124.8(5)
N54—C68—C44 123.6(5)
C5—C70—Sm1 174.6(4)
O3—C70—C5 117.0(5)
O3—C70—Sm1 57.7(3)
O42—C70—C5 122.3(5)
O42—C70—O3 120.7(5)
O42—C70—Sm1 63.1(3)
O1—C74—C44 117.3(5)
O14^{3_666}—C74—C44 118.3(5)
O14^{3_666}—C74—O1 124.4(5)
C62—N16—C15 117.7(5)
C20—N18—C57 117.2(5)
C68—N54—C25 117.0(5)
C66—O0AA—Sm2 144.9(4)
C74—O1—Sm1 162.8(4)
C30—O2—Sm2^{4_565} 137.8(4)
C70—O3—Sm1 96.4(3)
C70—O3—Sm2 136.3(3)
Sm2—O3—Sm1 103.39(14)
C41—O10—Sm1^{1_545} 138.8(3)
C41—O10—Sm2^{1_545} 95.8(3)
O33—Sm1—O3 85.19(13)
O33—Sm1—O10^{1_565} 69.39(13)
O33—Sm1—O14 82.34(14)
O33—Sm1—O21 140.50(13)
O33—Sm1—O25 141.34(14)
O33—Sm1—O42 70.35(13)
O33—Sm1—Sm2 76.05(9)
O42—Sm1—C70 24.77(13)
O42—Sm1—Sm2 82.52(9)
C41^{1_565}—Sm2—Sm1 59.55(10)
O0AA—Sm2—C41^{1_565} 151.37(14)
O0AA—Sm2—O2^{4_666} 71.54(13)
O0AA—Sm2—O3 95.95(14)
O0AA—Sm2—O10^{1_565} 140.62(12)
O0AA—Sm2—O16 87.34(13)
O0AA—Sm2—O40 70.97(13)
O0AA—Sm2—O44^{1_565} 145.82(14)
O0AA—Sm2—O48 79.88(14)
O0AA—Sm2—Sm1 125.91(10)
O2^{4_666}—Sm2—C41^{1_565} 91.11(13)
O2^{4_666}—Sm2—O44^{1_565} 111.76(12)
O2^{4_666}—Sm2—Sm1 64.09(9)
O3—Sm2—C41^{1_565} 97.75(14)
O3—Sm2—O2^{4_666} 66.67(12)
O3—Sm2—O10^{1_565} 76.06(12)
O3—Sm2—O40 77.81(13)
O3—Sm2—O44^{1_565} 116.95(13)
O3—Sm2—Sm1 38.93(9)
O10^{1_565}—Sm2—C41^{1_565} 25.76(13)
O10^{1_565}—Sm2—O2^{4_666} 69.93(12)
O10^{1_565}—Sm2—O44^{1_565} 50.01(12)
O10^{1_565}—Sm2—Sm1 37.23(9)
O11—Sm2—C41^{1_565} 71.57(14)
O11—Sm2—O0AA 137.02(14)
O11—Sm2—O2^{4_666} 129.02(13)
O11—Sm2—O3 68.76(13)
O11—Sm2—O10^{1_565} 76.53(13)
O11—Sm2—O16 87.33(13)
O11—Sm2—O40 66.65(14)
O11—Sm2—O44^{1_565} 69.03(13)
O11—Sm2—O48 138.24(14)

Sm1^{1_545}—O10—Sm2^{1_545} 103.06(13)	O11—Sm2—Sm1 65.88(9)
C37—O11—Sm2 138.5(3)	O16—Sm2—C41^{1_565} 94.01(13)
C74^{3_666}—O14—Sm1 143.8(4)	O16—Sm2—O2^{4_666} 142.74(12)
C66^{3_556}—O16—Sm2 137.5(4)	O16—Sm2—O3 148.15(13)
C37—O21—Sm1 127.0(3)	O16—Sm2—O10^{1_565} 119.73(12)
C30^{4_666}—O33—Sm1 125.8(3)	O16—Sm2—O40 73.38(13)
C70—O42—Sm1 92.1(3)	O16—Sm2—O44^{1_565} 69.88(12)
C41—O44—Sm2^{1_545} 92.3(3)	O16—Sm2—O48 73.50(14)
C70—Sm1—Sm2 59.67(11)	O16—Sm2—Sm1 146.47(9)
O1—Sm1—C70 175.08(14)	O40—Sm2—C41^{1_565} 136.65(14)
O1—Sm1—O3 156.87(13)	O40—Sm2—O2^{4_666} 124.17(13)
O1—Sm1—O10^{1_565} 83.11(13)	O40—Sm2—O10^{1_565} 140.55(13)
O1—Sm1—O14 78.73(13)	O40—Sm2—O44^{1_565} 122.57(13)
O1—Sm1—O21 79.49(13)	O40—Sm2—Sm1 110.51(9)
O1—Sm1—O25 104.87(15)	O44^{1_565}—Sm2—C41^{1_565} 24.27(13)
O1—Sm1—O33 99.41(14)	O44^{1_565}—Sm2—Sm1 81.43(9)
O1—Sm1—O42 152.02(13)	O48—Sm2—C41^{1_565} 73.17(14)
O1—Sm1—Sm2 121.24(10)	O48—Sm2—O2^{4_666} 72.80(13)
O3—Sm1—C70 25.91(13)	O48—Sm2—O3 138.30(13)
O3—Sm1—O42 50.67(12)	O48—Sm2—O10^{1_565} 81.41(13)
O3—Sm1—Sm2 37.68(9)	O48—Sm2—O40 136.34(14)
O10^{1_565}—Sm1—C70 96.65(14)	O48—Sm2—O44^{1_565} 69.59(13)
O10^{1_565}—Sm1—O3 77.30(12)	O48—Sm2—Sm1 112.85(10)

Selected Bond lengths of CP4

Table S7

C—O0AA 1.258(13)	Eu2—C38^{1_455} 2.949(11)
C0AA—C 1.533(15)	Eu2—C59 2.822(11)
C0AA—C5AA 1.399(15)	Eu2—O0AA 2.379(9)
C1—C6 1.216(16)	Eu2—O5 2.526(9)
C2AA—C3^{2_646} 1.525(15)	Eu2—O6 2.424(9)
C3—C2AA^{2_656} 1.525(15)	Eu2—O16^{1_455} 2.471(8)
C3—C10 1.390(14)	Eu2—O32 2.390(9)
C20—C43 1.426(16)	Eu2—O35 2.367(7)
C20—C76 1.355(15)	Eu2—O45 2.462(9)
C38—C51 1.504(15)	Eu2—O49 2.381(8)
C38—Eu2^{1_655} 2.949(11)	Eu2—O52^{1_455} 2.733(8)
C43—C5 1.405(14)	N1AA—C5 1.315(14)

C43—C78 1.498(15)	N1AA—C111 1.324(15)
C51—C65 1.411(15)	N2—C4AA 1.28(2)
C51—C107 1.414(15)	N2—C7 1.44(2)
C55—C76 1.501(15)	N2—C9 1.57(3)
C55—Eu1^{1_655} 2.869(11)	N3AA—C5AA 1.326(14)
C55—O73^{1_655} 1.249(14)	N3AA—C10 1.360(13)
C59—C89 1.496(15)	N25—C83 1.346(15)
C59—O5 1.271(12)	N25—C107 1.329(15)
C65—C89 1.391(16)	O1—C4AA 1.24(2)
C75—C0AA 1.359(15)	O6—C6 1.248(16)
C75—C3 1.388(16)	O12—C78 1.261(14)
C76—C111 1.405(14)	O16—C38 1.253(13)
C83—C89 1.414(15)	O16—Eu2^{1_655} 2.471(8)
Eu1—C55^{1_455} 2.869(12)	O18—C2AA 1.237(12)
Eu1—C78 2.986(11)	O35—C78 1.270(13)
Eu1—Eu2 4.083(2)	O41—C 1.259(13)
Eu1—O12 2.416(8)	O45—C59 1.266(13)
Eu1—O18 2.400(7)	O49—C2AA 1.270(13)
Eu1—O20 2.387(8)	O52—C38 1.252(12)
Eu1—O28 2.422(8)	O52—Eu1^{1_655} 2.386(7)
Eu1—O35 2.857(8)	O52—Eu2^{1_655} 2.733(8)
Eu1—O41 2.428(9)	O59—C55 1.291(13)
Eu1—O52^{1_455} 2.386(7)	O59—Eu1^{1_655} 2.476(8)
Eu1—O59^{1_455} 2.476(8)	O73—C55^{1_455} 1.249(14)
Eu1—O73 2.531(8)	

Selected Bond Angles of CP4
Table S8

O0AA—C—C0AA 115.6(9)	O52^{1_455}—Eu1—C78 99.5(3)
O0AA—C—O41 127.2(10)	O52^{1_455}—Eu1—Eu2 40.15(19)
O41—C—C0AA 117.2(9)	O52^{1_455}—Eu1—O12 123.4(3)
C5AA—C0AA—C 117.4(10)	O52^{1_455}—Eu1—O18 73.7(2)
C75—C0AA—C 123.3(10)	O52^{1_455}—Eu1—O28 79.0(3)
C75—C0AA—C5AA 119.1(11)	O52^{1_455}—Eu1—O35 74.6(2)
O18—C2AA—C3^{2_646} 117.0(9)	O52^{1_455}—Eu1—O41 78.8(3)
O18—C2AA—O49 129.1(10)	O52^{1_455}—Eu1—O59^{1_455} 92.4(3)
O49—C2AA—C3^{2_646} 114.0(9)	O52^{1_455}—Eu1—O73 136.7(3)
C10—C3—C2AA^{2_656} 117.1(10)	O59^{1_455}—Eu1—C55^{1_455} 26.7(3)
C75—C3—C2AA^{2_656} 124.5(10)	O59^{1_455}—Eu1—C78 139.9(3)
C75—C3—C10 118.4(11)	O59^{1_455}—Eu1—Eu2 123.58(18)

O1—C4AA—N2 128(2)
N1AA—C5—C43 124.7(11)
N3AA—C5AA—C0AA 121.1(10)
C1—C6—O6 129.7(14)
N3AA—C10—C3 120.6(10)
C76—C20—C43 118.9(10)
C51—C38—Eu2^{1_655} 169.3(7)
O16—C38—C51 118.1(9)
O16—C38—Eu2^{1_655} 55.7(5)
O52—C38—C51 118.6(10)
O52—C38—Eu2^{1_655} 67.8(6)
O52—C38—O16 123.3(10)
C5—C43—C20 116.7(10)
C5—C43—C78 120.7(10)
C20—C43—C78 122.0(10)
C65—C51—C38 121.1(9)
C65—C51—C107 118.1(10)
C107—C51—C38 120.8(10)
C76—C55—Eu1^{1_655} 167.2(8)
O59—C55—C76 117.8(10)
O59—C55—Eu1^{1_655} 59.4(6)
O73^{1_655}—C55—C76 122.1(9)
O73^{1_655}—C55—Eu1^{1_655} 61.8(6)
O73^{1_655}—C55—O59 120.1(11)
C89—C59—Eu2 170.2(7)
O5—C59—C89 119.7(10)
O5—C59—Eu2 63.5(6)
O45—C59—C89 116.8(9)
O45—C59—Eu2 60.6(6)
O45—C59—O5 123.5(10)
C89—C65—C51 118.1(10)
C0AA—C75—C3 120.4(11)
C20—C76—C55 119.7(9)
C20—C76—C111 118.0(11)
C111—C76—C55 122.0(10)
C43—C78—Eu1 168.1(8)
O12—C78—C43 117.6(9)
O12—C78—Eu1 51.7(6)
O12—C78—O35 123.4(10)
O35—C78—C43 118.9(10)
O35—C78—Eu1 71.8(6)
O59^{1_455}—Eu1—O35 142.1(3)
O59^{1_455}—Eu1—O73 52.1(2)
O73—Eu1—C55^{1_455} 25.8(3)
O73—Eu1—C78 96.3(3)
O73—Eu1—Eu2 136.46(18)
O73—Eu1—O35 116.3(2)
C38^{1_455}—Eu2—Eu1 59.0(2)
C59—Eu2—C38^{1_455} 121.8(3)
C59—Eu2—Eu1 136.4(2)
O0AA—Eu2—C38^{1_455} 71.9(3)
O0AA—Eu2—C59 73.5(3)
O0AA—Eu2—Eu1 65.7(2)
O0AA—Eu2—O5 71.7(3)
O0AA—Eu2—O6 138.3(3)
O0AA—Eu2—O16^{1_455} 75.3(3)
O0AA—Eu2—O32 137.4(3)
O0AA—Eu2—O45 75.1(3)
O0AA—Eu2—O52^{1_455} 69.4(3)
O5—Eu2—C38^{1_455} 138.8(3)
O5—Eu2—C59 26.8(3)
O5—Eu2—Eu1 119.67(18)
O5—Eu2—O52^{1_455} 140.6(3)
O6—Eu2—C38^{1_455} 87.0(3)
O6—Eu2—C59 89.2(3)
O6—Eu2—Eu1 132.0(2)
O6—Eu2—O5 108.3(3)
O6—Eu2—O16^{1_455} 71.4(3)
O6—Eu2—O45 73.2(3)
O6—Eu2—O52^{1_455} 105.0(3)
O16^{1_455}—Eu2—C38^{1_455} 24.8(3)
O16^{1_455}—Eu2—C59 101.3(3)
O16^{1_455}—Eu2—Eu1 83.16(18)
O16^{1_455}—Eu2—O5 124.6(3)
O16^{1_455}—Eu2—O52^{1_455} 49.8(2)
O32—Eu2—C38^{1_455} 149.0(3)
O32—Eu2—C59 83.5(3)
O32—Eu2—Eu1 116.8(2)
O32—Eu2—O5 71.7(3)
O32—Eu2—O6 74.7(3)
O32—Eu2—O16^{1_455} 145.6(3)
O32—Eu2—O45 99.5(3)

N25—C83—C89 122.9(11)	O32—Eu2—O52^{1_455} 138.6(3)
C65—C89—C59 120.6(9)	O35—Eu2—C38^{1_455} 101.9(3)
C65—C89—C83 119.2(11)	O35—Eu2—C59 111.2(3)
C83—C89—C59 120.1(10)	O35—Eu2—Eu1 43.1(2)
N25—C107—C51 124.0(12)	O35—Eu2—O0AA 73.5(3)
N1AA—C111—C76 125.0(11)	O35—Eu2—O5 85.5(3)
C55^{1_455}—Eu1—C78 120.3(3)	O35—Eu2—O6 147.5(3)
C55^{1_455}—Eu1—Eu2 138.4(2)	O35—Eu2—O16^{1_455} 125.3(3)
C78—Eu1—Eu2 59.4(2)	O35—Eu2—O32 82.5(3)
O12—Eu1—C55^{1_455} 101.5(3)	O35—Eu2—O45 134.3(3)
O12—Eu1—C78 24.2(3)	O35—Eu2—O49 79.6(3)
O12—Eu1—Eu2 83.4(2)	O35—Eu2—O52^{1_455} 77.4(2)
O12—Eu1—O28 146.3(3)	O45—Eu2—C38^{1_455} 98.9(3)
O12—Eu1—O35 49.1(2)	O45—Eu2—C59 26.6(3)
O12—Eu1—O41 85.2(3)	O45—Eu2—Eu1 139.1(2)
O12—Eu1—O59^{1_455} 126.4(3)	O45—Eu2—O5 53.2(3)
O12—Eu1—O73 76.0(3)	O45—Eu2—O16^{1_455} 76.1(3)
O18—Eu1—C55^{1_455} 74.2(3)	O45—Eu2—O52^{1_455} 120.4(3)
O18—Eu1—C78 73.3(3)	O49—Eu2—C38^{1_455} 77.1(3)
O18—Eu1—Eu2 65.95(19)	O49—Eu2—C59 153.3(3)
O18—Eu1—O12 79.8(3)	O49—Eu2—Eu1 68.2(2)
O18—Eu1—O28 133.6(3)	O49—Eu2—O0AA 133.0(3)
O18—Eu1—O35 68.6(2)	O49—Eu2—O5 143.7(3)
O18—Eu1—O41 133.4(3)	O49—Eu2—O6 72.0(3)
O18—Eu1—O59^{1_455} 73.6(3)	O49—Eu2—O16^{1_455} 90.6(3)
O18—Eu1—O73 72.8(3)	O49—Eu2—O32 73.6(3)
O20—Eu1—C55^{1_455} 81.0(3)	O49—Eu2—O45 145.2(3)
O20—Eu1—C78 96.4(3)	O49—Eu2—O52^{1_455} 67.5(3)
O20—Eu1—Eu2 139.6(2)	O52^{1_455}—Eu2—C38^{1_455} 25.1(2)
O20—Eu1—O12 78.1(3)	O52^{1_455}—Eu2—C59 137.6(3)
O20—Eu1—O18 142.4(3)	O52^{1_455}—Eu2—Eu1 34.26(15)
O20—Eu1—O28 70.8(3)	C5—N1AA—C111 116.4(9)
O20—Eu1—O35 115.6(3)	C4AA—N2—C7 134(2)
O20—Eu1—O41 74.1(3)	C4AA—N2—C9 117.1(17)
O20—Eu1—O52^{1_455} 143.7(3)	C7—N2—C9 108.9(14)
O20—Eu1—O59^{1_455} 96.1(3)	C5AA—N3AA—C10 120.4(10)
O20—Eu1—O73 72.6(3)	C107—N25—C83 117.8(10)
O28—Eu1—C55^{1_455} 86.4(3)	C—O0AA—Eu2 141.6(7)
O28—Eu1—C78 149.0(3)	C59—O5—Eu2 89.7(7)
O28—Eu1—Eu2 112.3(2)	C6—O6—Eu2 134.9(9)
O28—Eu1—O35 137.4(3)	C78—O12—Eu1 104.2(7)

O28—Eu1—O41 74.3(3)	C38—O16—Eu2^{1_655} 99.5(6)
O28—Eu1—O59^{1_455} 70.8(3)	C2AA—O18—Eu1 138.7(7)
O28—Eu1—O73 105.9(3)	C78—O35—Eu1 83.2(6)
O35—Eu1—C55^{1_455} 135.5(3)	C78—O35—Eu2 172.4(7)
O35—Eu1—C78 25.0(2)	Eu2—O35—Eu1 102.4(3)
O35—Eu1—Eu2 34.49(15)	C—O41—Eu1 133.9(7)
O41—Eu1—C55^{1_455} 152.3(3)	C59—O45—Eu2 92.8(6)
O41—Eu1—C78 75.1(3)	C2AA—O49—Eu2 133.7(7)
O41—Eu1—Eu2 68.7(2)	C38—O52—Eu1^{1_655} 162.5(7)
O41—Eu1—O35 68.3(3)	C38—O52—Eu2^{1_655} 87.1(6)
O41—Eu1—O59^{1_455} 145.0(3)	Eu1^{1_655}—O52—Eu2^{1_655} 105.6(3)
O41—Eu1—O73 144.4(3)	C55—O59—Eu1^{1_655} 93.9(7)
O52^{1_455}—Eu1—C55^{1_455} 117.2(3)	C55^{1_455}—O73—Eu1 92.4(6)

Selected Bond lengths of CP5
Table S9

C4—H4 0.9300	Gd1—O22 2.368(10)
C4—N3^{8_654} 1.324(16)	Gd1—O25 2.360(9)
C5—C4 1.418(18)	Gd1—O38 2.385(9)
C5—C6^{3_675} 1.389(17)	Gd1—O39 2.379(9)
C6—C5^{2_765} 1.389(17)	Gd1—O40 2.483(10)
C6—H6 0.9300	Gd2—C33 2.765(14)
C7—C6 1.371(16)	Gd2—N15 2.699(13)
C7—C8 1.36(2)	Gd2—N29^{9_664} 2.633(12)
C8—H8 0.9300	Gd2—O10 2.308(10)
C8—N3^{9_664} 1.331(17)	Gd2—O13 2.345(10)
C9—C5 1.508(17)	Gd2—O23 2.374(10)
C12—C7 1.478(17)	Gd2—O26 2.317(10)
C16—H16 0.9300	Gd2—O34 2.418(11)
C16—N15^{6_565} 1.322(18)	Gd2—O35 2.475(10)
C17—C16 1.33(2)	N3—C4^{6_565} 1.324(16)
C17—C18 1.382(19)	N3—C8^{5_655} 1.331(17)
C17—C21^{2_655} 1.502(16)	N15—C16^{8_654} 1.322(18)
C18—H18 0.9300	N15—C20 1.346(18)
C19—C18 1.388(18)	N29—C28^{4} 1.369(19)
C19—C20^{6_565} 1.411(19)	N29—Gd2^{5_655} 2.633(12)
C20—C19^{8_654} 1.411(19)	O0AA—H0AA 0.8501
C20—H20 0.9300	O0AA—H0AB 0.8501
C21—C17^{3_665} 1.502(16)	O1—H1A 0.8501

C24—C19 1.530(16)	O1—H1B 0.8498
C27—C28 1.32(2)	O10—C9 1.229(18)
C27—C33 1.529(19)	O11—C9 1.27(2)
C28—H28 0.9300	O13—C12 1.256(17)
C28—N29^{7_444} 1.369(19)	O14—C12 1.241(18)
C30—H30 0.9300	O22—C21 1.283(17)
C30—N29 1.292(19)	O23—C21 1.217(19)
C31—C30 1.353(19)	O25—C24 1.230(17)
C31—C32^{4} 1.337(19)	O26—C24 1.281(19)
C31—C36 1.516(17)	O34—C33 1.211(19)
C32—C27 1.398(18)	O35—C33 1.306(17)
C32—C31^{7_444} 1.337(19)	O38—C36 1.261(16)
C32—H32 0.9300	O39—H39A 1.1680
C36—O37 1.245(18)	O39—H39B 1.1616
Gd1—N3 2.667(11)	O40—H40A 0.9700
Gd1—O11 2.324(10)	O40—H40B 0.9682
Gd1—O14 2.354(10)	

Selected Bond Angles of CP5

Table S10

C3AA—C—C2AA 121.1(13)	O1AA—Gd1—N6 113.1(5)
C3AA—C—C15 119.3(12)	O1AA—Gd1—O8 53.4(4)
C15—C—C2AA 119.6(12)	O8—Gd1—C1AA 28.2(4)
C0BA—C0AA—C5AA 121.9(13)	O8—Gd1—N3^{9_564} 100.6(5)
C14—C0AA—C0BA 116.8(12)	O8—Gd1—N6 73.8(4)
C14—C0AA—C5AA 121.2(13)	O15—Gd1—C1AA 163.5(4)
C0AA—C0BA—C9^{2_665} 119.6(12)	O15—Gd1—N3^{9_564} 75.1(4)
C0AA—C0BA—H0BA 120.3	O15—Gd1—N6 76.2(4)
C9^{2_665}—C0BA—H0BA 120.2	O15—Gd1—O1AA 144.3(4)
C6AA—C1AA—Gd1 163.6(10)	O15—Gd1—O8 150.0(4)
O1AA—C1AA—C6AA 121.4(13)	O15—Gd1—O31 78.8(4)
O1AA—C1AA—Gd1 61.2(8)	O21—Gd1—C1AA 101.0(4)
O1AA—C1AA—O8 122.6(14)	O21—Gd1—N3^{9_564} 76.0(5)
O8—C1AA—C6AA 116.0(13)	O21—Gd1—N6 150.5(5)
O8—C1AA—Gd1 63.5(7)	O21—Gd1—O1AA 77.9(5)
O17—C2AA—C 115.2(12)	O21—Gd1—O8 128.7(4)
O31—C2AA—C 118.7(13)	O21—Gd1—O15 79.9(4)
O31—C2AA—O17 126.1(13)	O21—Gd1—O31 121.1(5)
C—C3AA—H3AA 117.2	O31—Gd1—C1AA 113.7(4)
N3—C3AA—C 125.7(13)	O31—Gd1—N3^{9_564} 145.4(4)

N3—C3AA—H3AA 117.1
C6—C4AA—C6AA 119.0(13)
C6—C4AA—H4AA 120.5
C6AA—C4AA—H4AA 120.5
C9—C5—H5 118.7
N12^{3_565}—C5—C9 122.6(12)
N12^{3_565}—C5—H5 118.7
O15—C5AA—C0AA 116.8(13)
O30—C5AA—C0AA 118.2(13)
O30—C5AA—O15 124.9(13)
C4AA—C6—C13^{2_765} 116.5(13)
C4AA—C6—C16 122.3(12)
C13^{2_765}—C6—C16 121.1(12)
C4AA—C6AA—C1AA 117.4(13)
C8AA^{2_765}—C6AA—C1AA 122.9(13)
C8AA^{2_765}—C6AA—C4AA 119.0(13)
C8—C7AA—H7AA 120.0
N3—C7AA—C8 120.0(13)
N3—C7AA—H7AA 120.0
C7AA—C8—C17 116.8(12)
C15—C8—C7AA 119.5(12)
C15—C8—C17 123.7(12)
C6AA^{3_675}—C8AA—H8AA 118.3
C6AA^{3_675}—C8AA—N6 123.3(14)
N6—C8AA—H8AA 118.5
C0BA^{3_565}—C9—C5 117.4(11)
C0BA^{3_565}—C9—C18 121.7(12)
C5—C9—C18 120.9(13)
C6^{3_675}—C13—H13 116.1
N6—C13—C6^{3_675} 127.8(14)
N6—C13—H13 116.1
C0AA—C14—H14 116.8
N12—C14—C0AA 126.5(12)
N12—C14—H14 116.7
C—C15—C8 117.6(14)
C—C15—H15 121.2
C8—C15—H15 121.2
O3AA—C16—C6 115.6(12)
O4—C16—C6 119.7(12)
O4—C16—O3AA 124.4(13)
O0AA—C17—C8 113.3(12)
O31—Gd1—N6 70.7(4)
O31—Gd1—O1AA 136.8(4)
O31—Gd1—O8 90.8(4)
O2AA—Gd2—N12^{5_665} 70.7(4)
O2AA—Gd2—O3AA^{4_455} 105.2(5)
O2AA—Gd2—O9AA 70.3(4)
O3AA^{4_455}—Gd2—N12^{5_665} 75.8(4)
O3AA^{4_455}—Gd2—O9AA 72.6(4)
O9AA—Gd2—N12^{5_665} 119.9(4)
O12^{2_765}—Gd2—N12^{5_665} 74.2(4)
O12^{2_765}—Gd2—O2AA 82.6(4)
O12^{2_765}—Gd2—O3AA^{4_455} 144.2(4)
O12^{2_765}—Gd2—O9AA 140.6(4)
O12^{2_765}—Gd2—O17 76.0(5)
O17—Gd2—N12^{5_665} 75.2(4)
O17—Gd2—O2AA 143.6(4)
O17—Gd2—O3AA^{4_455} 77.9(4)
O17—Gd2—O9AA 141.0(4)
O22—Gd2—N12^{5_665} 138.1(4)
O22—Gd2—O2AA 77.2(4)
O22—Gd2—O3AA^{4_455} 140.0(4)
O22—Gd2—O9AA 71.0(4)
O22—Gd2—O12^{2_765} 75.6(4)
O22—Gd2—O17 123.9(4)
O22—Gd2—O30 76.3(4)
O30—Gd2—N12^{5_665} 144.6(4)
O30—Gd2—O2AA 139.6(4)
O30—Gd2—O3AA^{4_455} 77.6(4)
O30—Gd2—O9AA 72.4(4)
O30—Gd2—O12^{2_765} 119.0(4)
O30—Gd2—O17 76.8(4)
C3AA—N3—C7AA 117.5(14)
C3AA—N3—Gd1^{5_665} 126.0(10)
C7AA—N3—Gd1^{5_665} 116.5(9)
C8AA—N6—Gd1 119.8(10)
C13—N6—C8AA 114.4(12)
C13—N6—Gd1 123.5(11)
C5^{2_665}—N12—C14 116.9(11)
C5^{2_665}—N12—Gd2^{9_564} 124.5(8)
C14—N12—Gd2^{9_564} 118.4(8)
C17—O0AA—Gd1^{3_675} 139.8(10)

O12—C17—C8 117.9(13)	H1A—O1—H1B 109.3
O12—C17—O0AA 128.8(12)	C1AA—O1AA—Gd1 93.1(9)
O21—C18—C9 119.5(15)	Gd2—O2AA—H2AA 119.2
O21—C18—O22 124.3(13)	Gd2—O2AA—H2AB 119.3
O22—C18—C9 116.2(12)	H2AA—O2AA—H2AB 97.8
$N3^{9\_564}$—Gd1—C1AA 89.1(4)	C16—O3AA—$Gd2^{7\_544}$ 140.4(10)
N6—Gd1—C1AA 97.2(4)	C1AA—O8—Gd1 88.2(8)
N6—Gd1—$N3^{9\_564}$ 81.3(4)	Gd2—O9AA—H9AA 112.3
$O0AA^{2\_765}$—Gd1—C1AA 68.6(5)	Gd2—O9AA—H9AB 112.9
$O0AA^{2\_765}$—Gd1—$N3^{9\_564}$ 141.2(4)	H9AA—O9AA—H9AB 105.9
$O0AA^{2\_765}$—Gd1—N6 131.0(5)	C17—O12—$Gd2^{3\_675}$ 145.3(10)
$O0AA^{2\_765}$—Gd1—O1AA 74.3(5)	C5AA—O15—Gd1 139.5(10)
$O0AA^{2\_765}$—Gd1—O8 74.7(4)	C2AA—O17—Gd2 152.6(10)
$O0AA^{2\_765}$—Gd1—O15 127.1(4)	C18—O21—Gd1 158.7(12)
$O0AA^{2\_765}$—Gd1—O21 77.7(5)	C18—O22—Gd2 134.6(9)
$O0AA^{2\_765}$—Gd1—O31 73.3(4)	C5AA—O30—Gd2 149.0(9)
O1AA—Gd1—C1AA 25.7(4)	C2AA—O31—Gd1 136.4(10)
O1AA—Gd1—$N3^{9\_564}$ 72.6(4)	

Selected Bond lengths of CP6
Table S11

C0AA—C1 1.34(3)	$Er1—O20^{7\_566}$ 2.402(4)
C0AA—C2 1.25(2)	Er1—O29 2.335(4)
C1AA—C5 1.363(7)	Er1—O34 2.534(3)
C2AA—C0AA 1.483(9)	$Er1—O34^{5\_676}$ 2.271(3)
C3—C5 1.384(7)	N23—C1AA 1.340(7)
C3—C9 1.382(7)	N23—C4 1.350(6)
C9—C4 1.387(7)	O0AA—C2AA 1.234(7)
C9—C15 1.521(6)	O1—C32 1.263(6)
C32—C5 1.494(7)	$O1—Er1^{7\_566}$ 2.410(4)
$C32—Er1^{7\_566}$ 2.768(5)	O8—C15 1.249(6)
Er1—C2AA 2.837(6)	O20—C32 1.253(6)
$Er1—C32^{7\_566}$ 2.768(5)	$O20—Er1^{7\_566}$ 2.402(4)
Er1—O0AA 2.385(4)	O30—C15 1.245(6)
$Er1—O1^{7\_566}$ 2.410(4)	O34—C2AA 1.267(6)
Er1—O6 2.283(4)	$O34—Er1^{5\_676}$ 2.271(3)

Er1—O8	2.220(4)

Selected Bond Angles of CP6
Table S12

C1—C0AA—C2AA	107.9(12)
C2—C0AA—C1	83.4(15)
C2—C0AA—C2AA	118.4(11)
N23—C1AA—C5	124.3(5)
C0AA—C2AA—Er1	178.1(6)
O0AA—C2AA—C0AA	122.2(5)
O0AA—C2AA—Er1	56.3(3)
O0AA—C2AA—O34	119.6(5)
O34—C2AA—C0AA	118.2(6)
O34—C2AA—Er1	63.3(3)
C9—C3—C5	119.1(5)
N23—C4—C9	123.2(5)
C1AA—C5—C3	118.6(5)
C1AA—C5—C32	119.4(4)
C3—C5—C32	122.0(5)
C3—C9—C4	118.2(5)
C3—C9—C15	123.1(4)
C4—C9—C15	118.7(4)
O8—C15—C9	117.1(4)
O30—C15—C9	116.3(5)
O30—C15—O8	126.5(5)
C5—C32—Er1^{7_566}	175.7(3)
O1—C32—C5	119.8(5)
O1—C32—Er1^{7_566}	60.4(3)
O20—C32—C5	119.7(5)
O20—C32—Er1^{7_566}	60.1(3)
O20—C32—O1	120.5(5)
C32^{7_566}—Er1—C2AA	100.83(17)
O0AA—Er1—C2AA	25.50(13)
O0AA—Er1—C32^{7_566}	103.31(15)
O0AA—Er1—O1^{7_566}	78.54(14)
O0AA—Er1—O20^{7_566}	126.78(15)
O0AA—Er1—O34	52.02(12)
O1^{7_566}—Er1—C2AA	73.72(15)
O1^{7_566}—Er1—C32^{7_566}	27.12(14)
O1^{7_566}—Er1—O34	72.25(12)
O6—Er1—O20^{7_566}	84.76(16)
O6—Er1—O29	103.12(19)
O6—Er1—O34	123.59(12)
O8—Er1—C2AA	155.52(16)
O8—Er1—C32^{7_566}	103.64(15)
O8—Er1—O0AA	142.41(15)
O8—Er1—O1^{7_566}	130.74(13)
O8—Er1—O6	83.03(15)
O8—Er1—O20^{7_566}	76.77(13)
O8—Er1—O29	79.89(15)
O8—Er1—O34	147.52(14)
O8—Er1—O34^{5_676}	90.17(14)
O20^{7_566}—Er1—C2AA	127.70(15)
O20^{7_566}—Er1—C32^{7_566}	26.87(14)
O20^{7_566}—Er1—O1^{7_566}	53.98(12)
O20^{7_566}—Er1—O34	120.03(13)
O29—Er1—C2AA	76.18(17)
O29—Er1—C32^{7_566}	168.67(18)
O29—Er1—O0AA	78.81(16)
O29—Er1—O1^{7_566}	148.16(14)
O29—Er1—O20^{7_566}	154.25(15)
O29—Er1—O34	76.21(15)
O34—Er1—C2AA	26.52(13)
O34^{5_676}—Er1—C2AA	92.86(14)
O34—Er1—C32^{7_566}	96.17(14)
O34^{5_676}—Er1—C32^{7_566}	83.99(14)
O34^{5_676}—Er1—O0AA	118.33(12)
O34^{5_676}—Er1—O1^{7_566}	86.11(13)
O34^{5_676}—Er1—O6	168.05(14)
O34^{5_676}—Er1—O20^{7_566}	84.11(15)
O34^{5_676}—Er1—O29	85.24(18)
O34^{5_676}—Er1—O34	66.36(13)
C1AA—N23—C4	116.5(4)
C2AA—O0AA—Er1	98.2(3)
C32—O1—Er1^{7_566}	92.4(3)
C15—O8—Er1	166.5(4)

O6—Er1—C2AA 97.40(15)	C32—O20—Er1^{7_566} 93.1(3)
O6—Er1—C32^{7_566} 88.06(15)	C2AA—O34—Er1^{5_676} 156.0(4)
O6—Er1—O0AA 72.21(13)	C2AA—O34—Er1 90.2(3)
O6—Er1—O1^{7_566} 90.88(13)	Er1^{5_676}—O34—Er1 113.63(13)

Tables: Hydrogen bonds for CP **1-6** [Å and °].

Selected hydrogen-bond parameters **CP1**

Table S13

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
O3—H3A···N42^{i}	0.89	2.03	2.86 (2)	155.2
O26—H26···N30^{ii}	0.82	1.72	2.51 (2)	162.7
O27—H27B···O25^{iii}	0.85	2.58	2.83 (2)	98.0
O52—H52B···O50^{iv}	0.94	2.30	2.78 (2)	111.3
O53—H53A···O55^{v}	0.91	1.93	2.81 (2)	163.6

Symmetry code(s): (i) *x*−1, *y*, *z*−1; (ii) *x*−1, *y*−1, *z*; (iii) *x*+1, *y*+1, *z*; (iv) *x*−1, *y*, *z*; (v) *x*, *y*, *z*−1.

Selected hydrogen-bond parameters **CP2**

Table S14

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
O27—H27A···N1$^{1\text{-}655}$	0.85	2.05	2.809 (6)	148.0
O27—H27B...O3	0.85	2.16	2.750 (10)	126.2
O27—H27B···O25^{iii}	0.85	2.04	2.751 (8)	140
O27—H27B...O3	0.85	2.07	2.779 (11)	139.9

Symmetry code(s): (i) *x*−1, *y*, *z*−1; (ii) *x*−1, *y*−1, *z*; (iii) *x*+1, *y*+1, *z*; (iv) *x*−1, *y*, *z*; (v) *x*, *y*, *z*−1.

Selected hydrogen-bond parameters **CP3**

Table S15

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
O27—H27B...N^{34_565}	0.88	1.94	2.7689 (6)	157.8
O28—H28A...O42	0.87	2.19	2.860 (6)	133.6
O28—H28B...O10^{3_656}	0.87	2.01	2.788 (5)	148.5

Symmetry code(s): (i) *x*−1, *y*, *z*−1; (ii) *x*−1, *y*−1, *z*; (iii) *x*+1, *y*+1, *z*; (iv) *x*−1, *y*, *z*; (v) *x*, *y*, *z*−1.

Selected hydrogen-bond parameters **CP4**

Table S16

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
O30—H30B...O39 $^{3\_667}$	0.90	2.69	2.821(15)	89.0
O43—H43B...N6^{3_666}	0.88	2.16	2.809 (14)	131.0
O46—H46A...O43 $^{3\_766}$	0.85	2.00	2.791(18)	155.4

Symmetry code(s): (i) *x*−1, *y*, *z*−1; (ii) *x*−1, *y*−1, *z*; (iii) *x*+1, *y*+1, *z*; (iv) *x*−1, *y*, *z*; (v) *x*, *y*, *z*−1.

Selected hydrogen-bond parameters **CP5**

Table S17

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
C7AA—H7AA...O1AA^{5_665}	0.93	2.24	2.880(16)	125.4
O2AA—H2AA...O4^{6_565}	1.12	1.90	2.772(6)	131.3

Symmetry code(s): (i) *x*−1, *y*, *z*−1; (ii) *x*−1, *y*−1, *z*; (iii) *x*+1, *y*+1, *z*; (iv) *x*−1, *y*, *z*; (v) *x*, *y*, *z*−1.

Selected hydrogen-bond parameters **CP6**

Table S18

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
O1W-H12W···O3[1]	2.922(5)	2.24	2.63(7)	131.3
O1W-H11W···O4[2]	2.594(5)	1.80(4)	2.772(6)	164
O2W-H21W···O2[3]	2.887(5)	2.07(4)	2.07(4)	179
O1W-H12W···O1W[4]	2.977(6)	2.052(4)	2.57(8)	111
O2W-H22W···N1[5]	2.672(5)	1.874(4)	1.98(5)	143

Symmetry code(s): (i) -x+1/2+1,-y+1/2+1,-z+ (ii) x+1/2,-y+1/2+1,+z-1/2 (iii) -x+2,-y+1,-z+1 (iv) -x+2,+y,-z+1/2 (v) x,-y+1,+z-1/2