

Electronic Supplementary Information

**2,5-furandicarboxylic acid as a linker for lanthanide coordination
polymers: the role of heteroaromatic π - π stacking and hydrogen
bonding**

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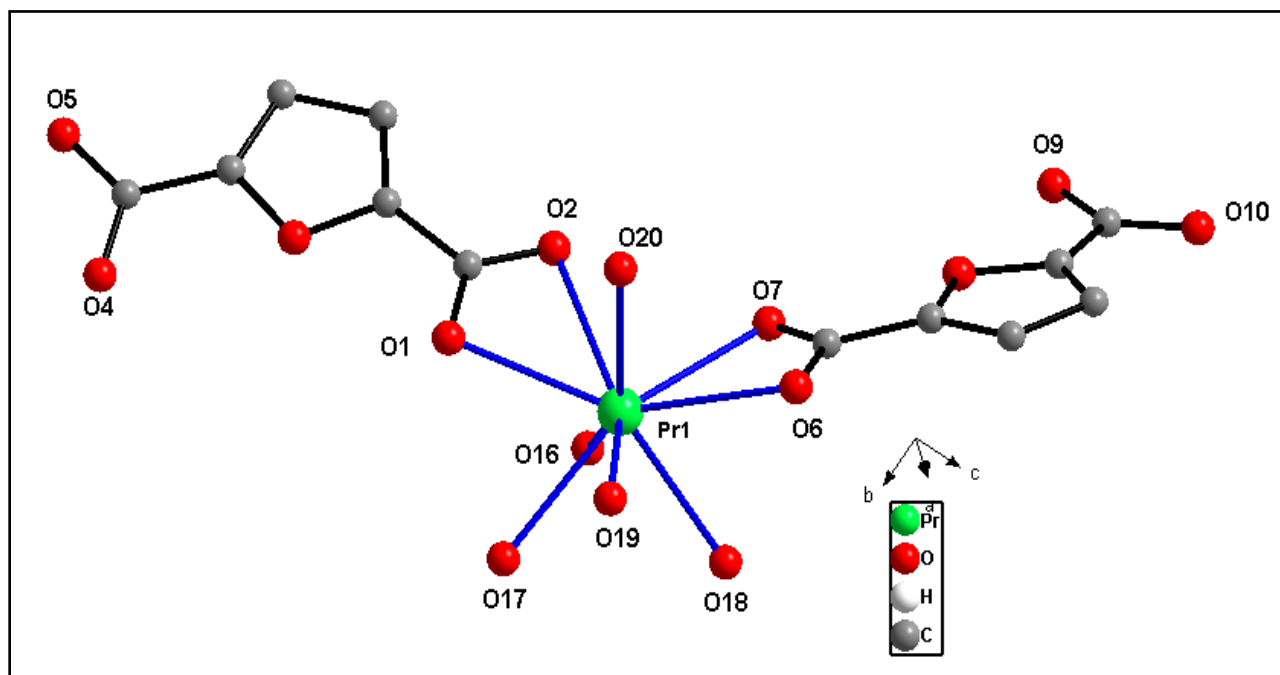


Fig. S1 Coordination environment of Pr01 in CP 1.

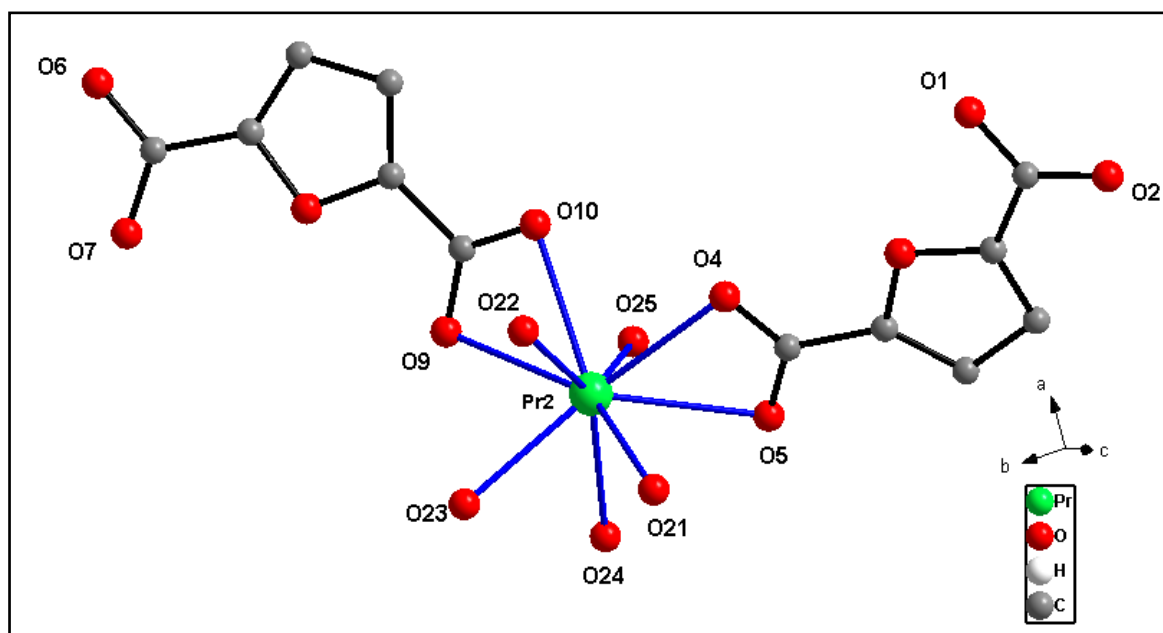


Fig. S2 Coordination environment of Pr02 in CP 1.

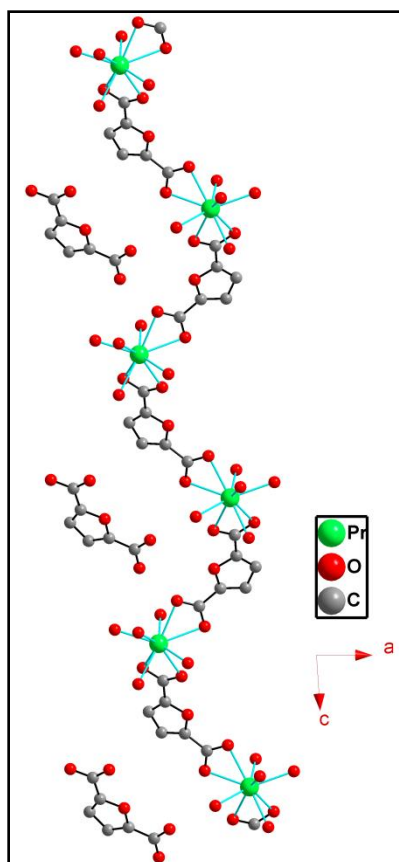


Fig. S3 Linear extension of 1DCP 1 along b-axis.

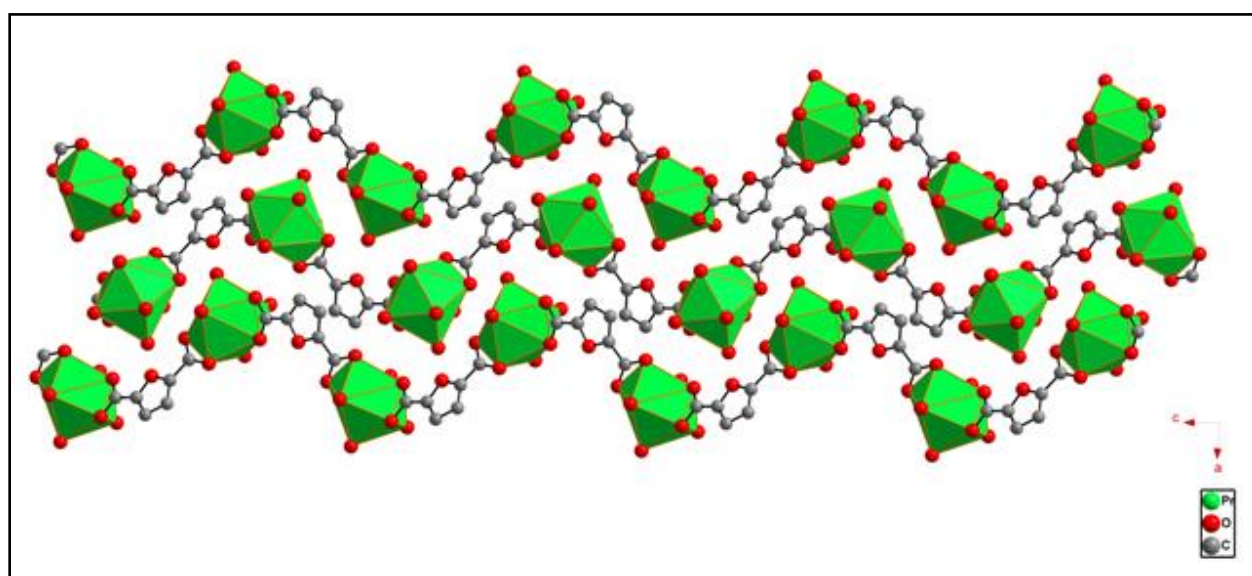


Fig. S4 Packing of CP1 along b-axis.

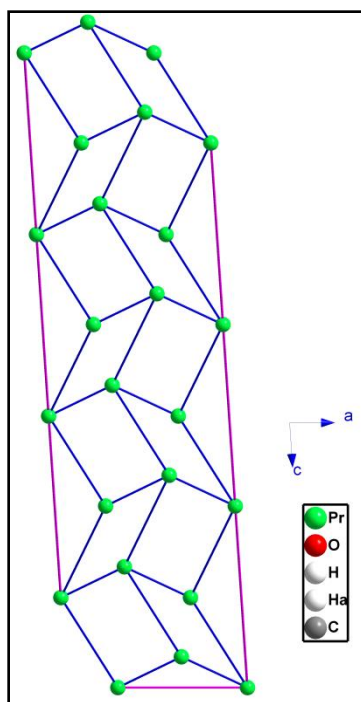


Fig. S5 2D (4,4)-Rhombic topological view along b-axis.

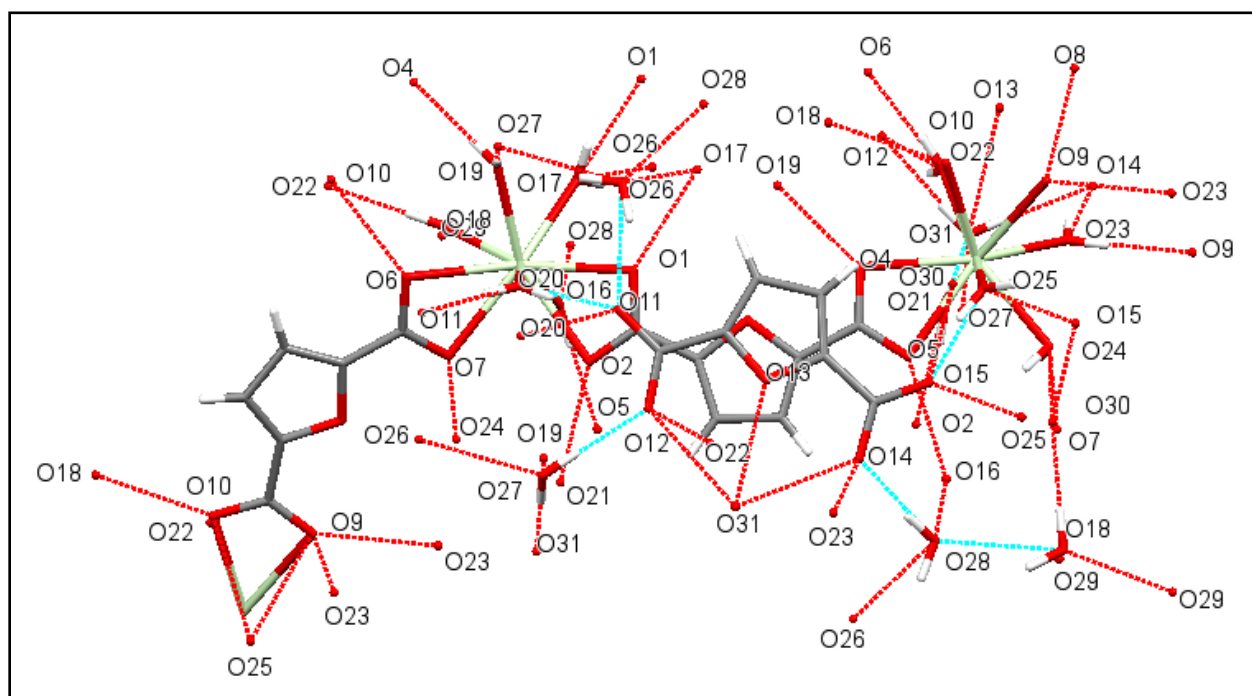


Fig. S6 Number and positions of hydrogen bonds in CP 1.

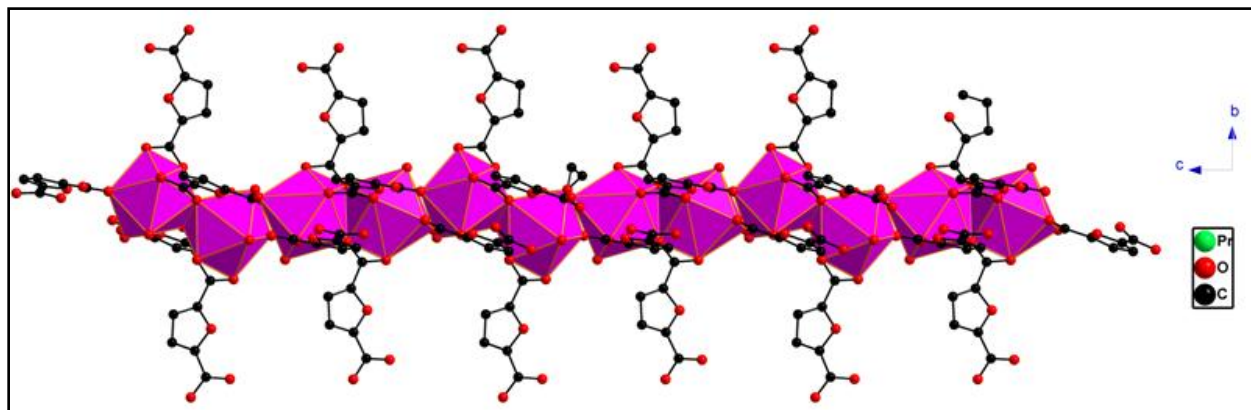


Fig. S7 Polyheral packing arrangement of CP 2 when viewed along a-axis.

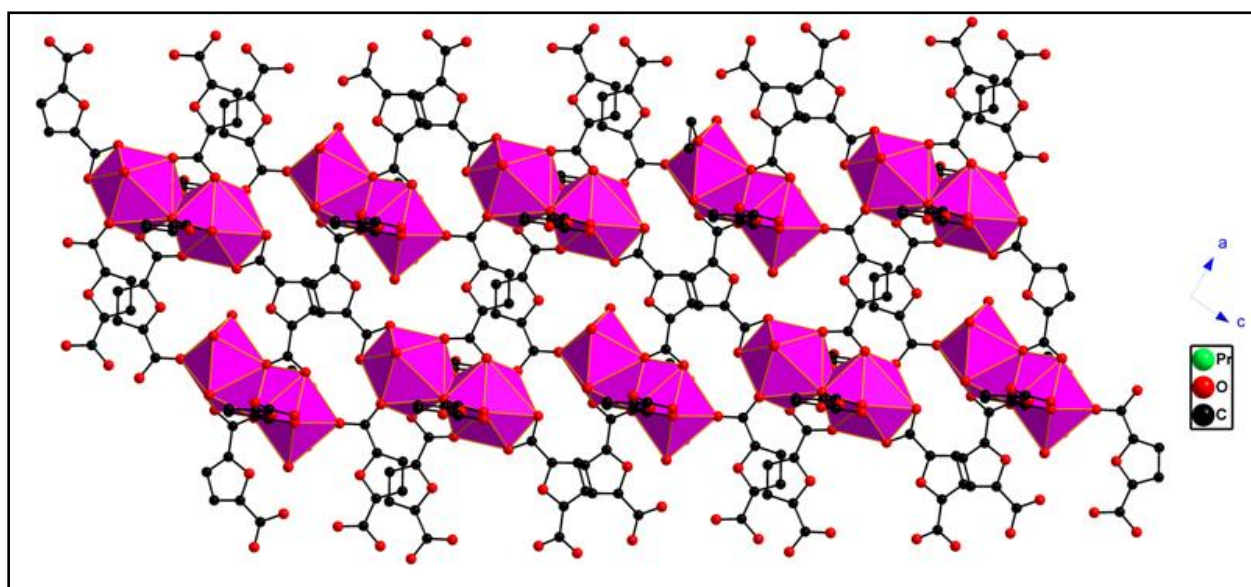


Fig. S8 Polyheral packing arrangements of CP 2 when viewed along b-axis.

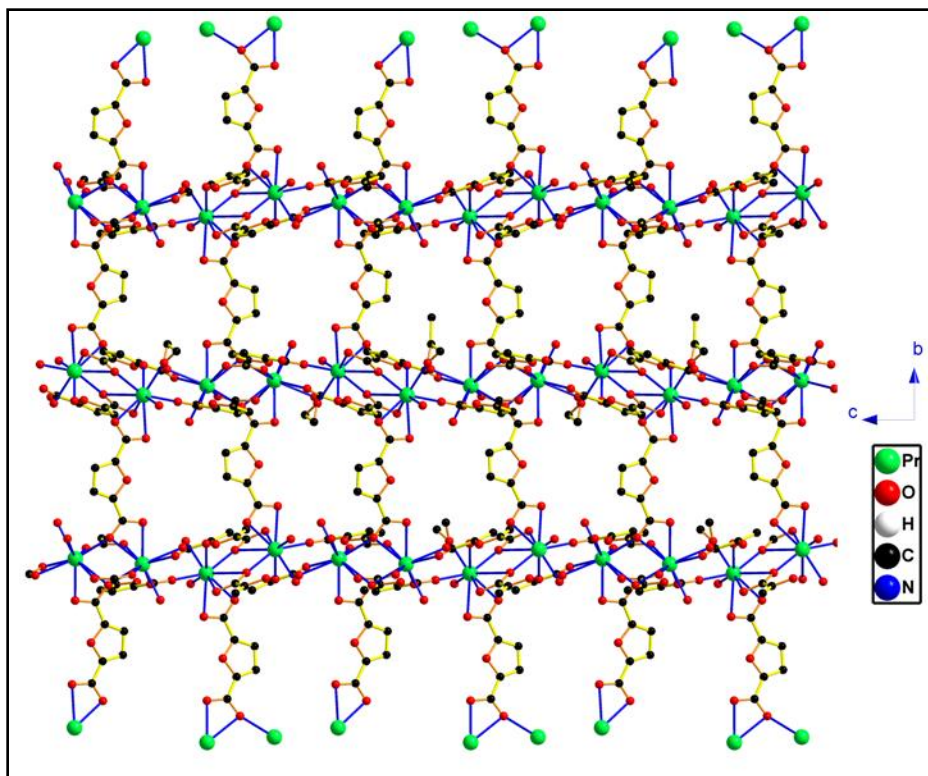


Fig. S9 Packing in CP2 when view along a-axis.

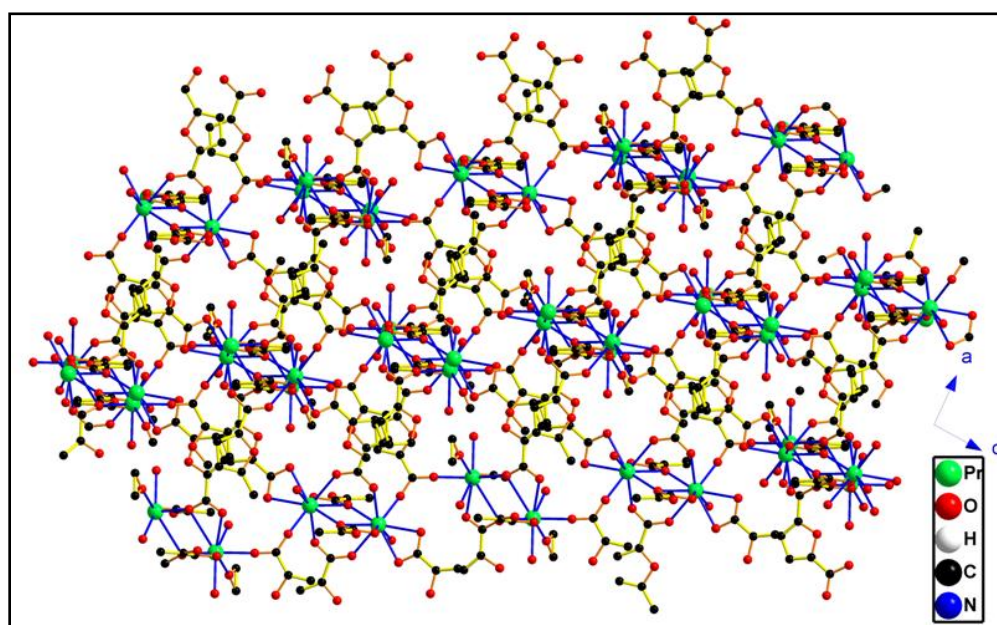


Fig. S10 Packing in CP2 when view along b-axis.

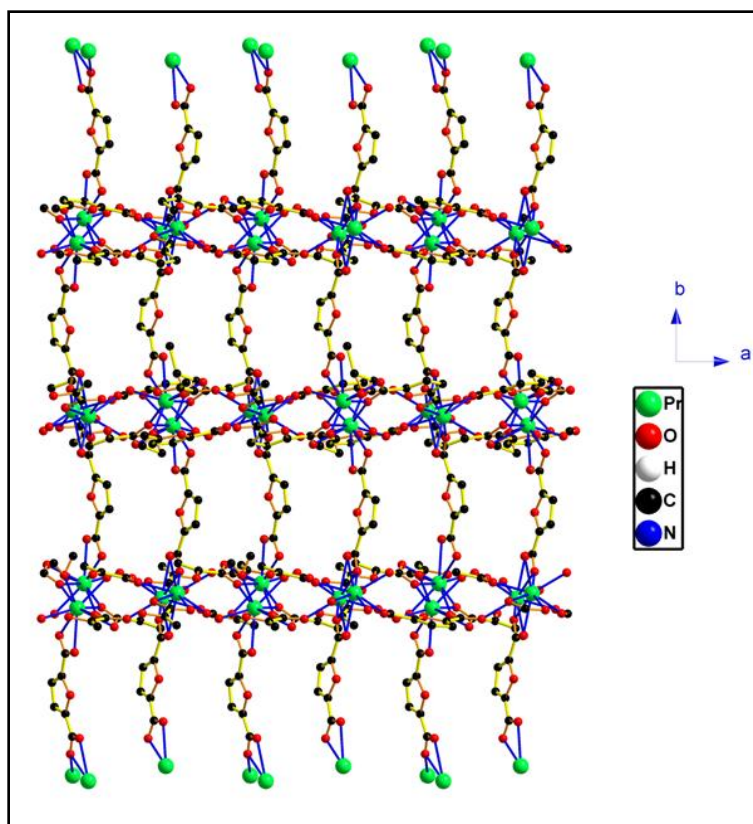


Fig. S11 Packing in CP2 when view along c-axis.

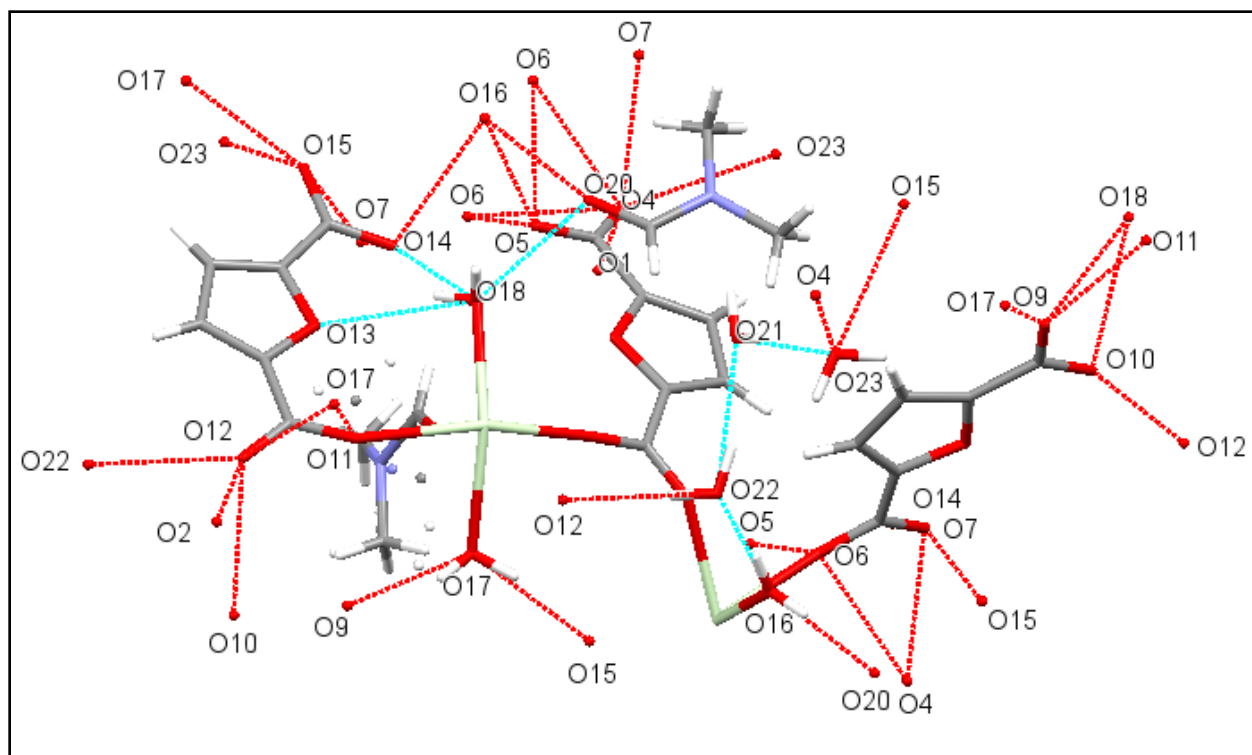


Fig. S12 Number and positions of Hydrogen bonds in asymmetric unit of CP 2.

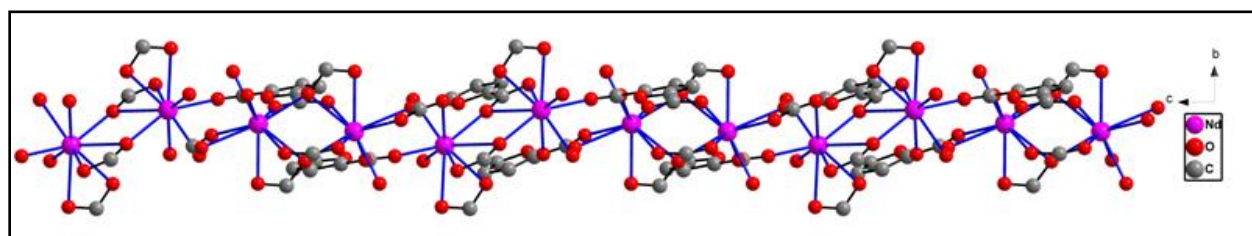


Fig. S13 Packing in CP 5 when view along a-axis.

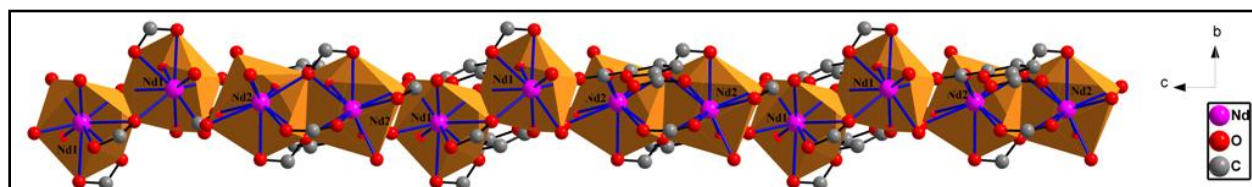


Fig. S14 Polyheral packing arrangement of CP 5 when viewed along a-axis.

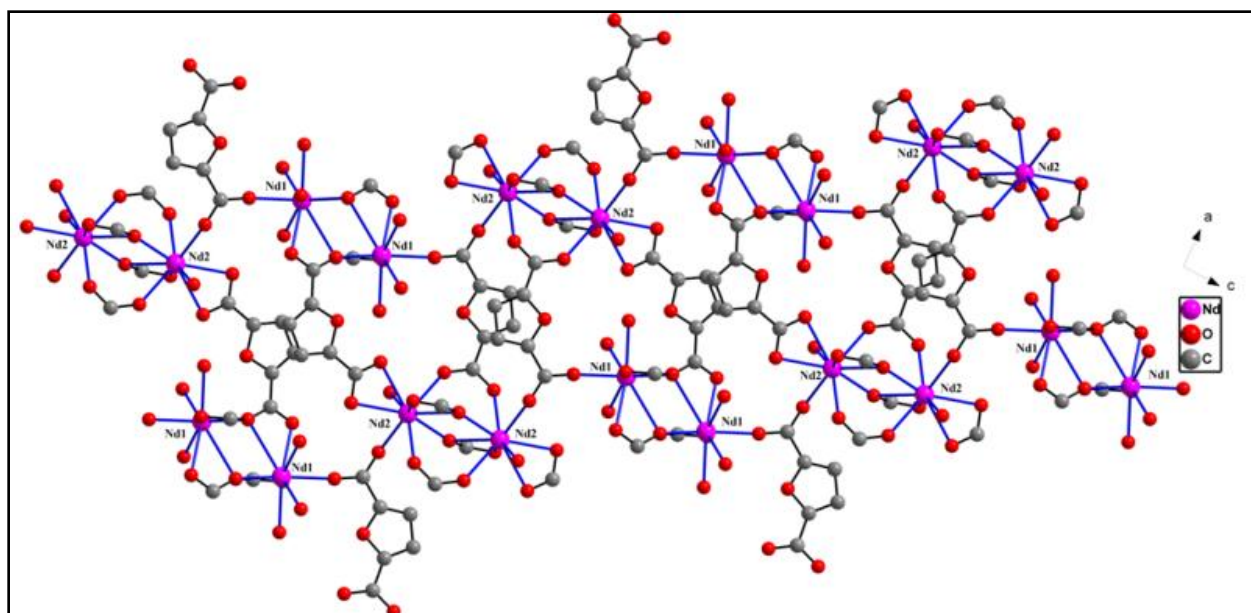


Fig. S15 Packing in CP 5 when view along b-axis.

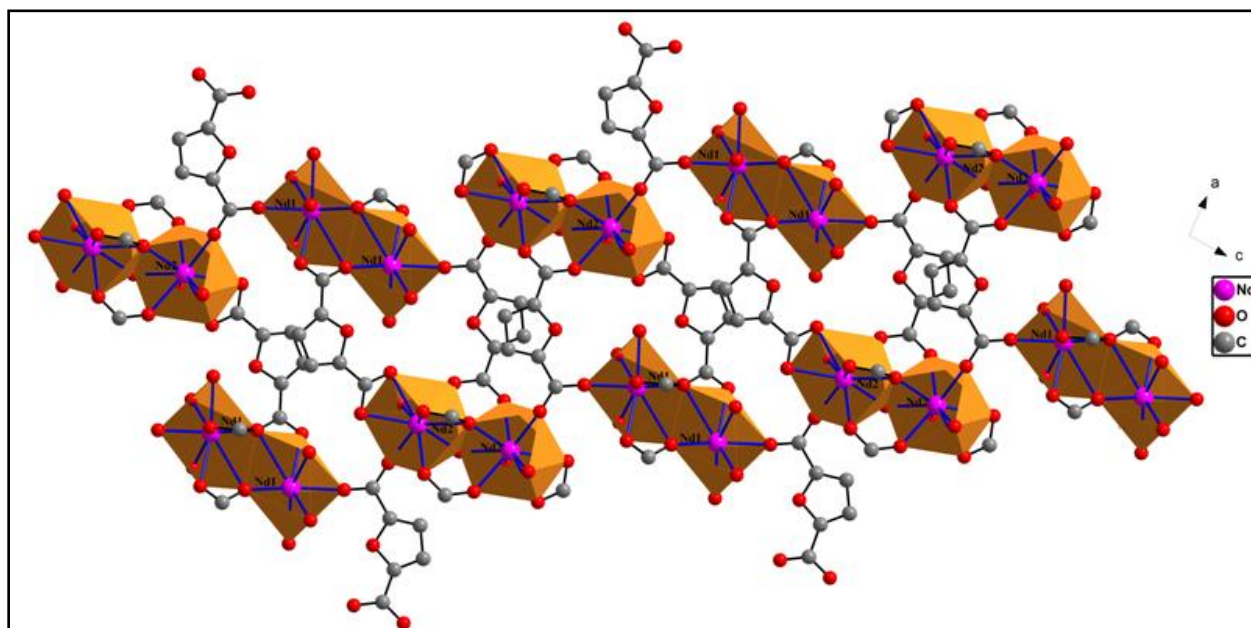


Fig. S16 Polyhedral packing arrangement of CP 5 when viewed along b-axis.

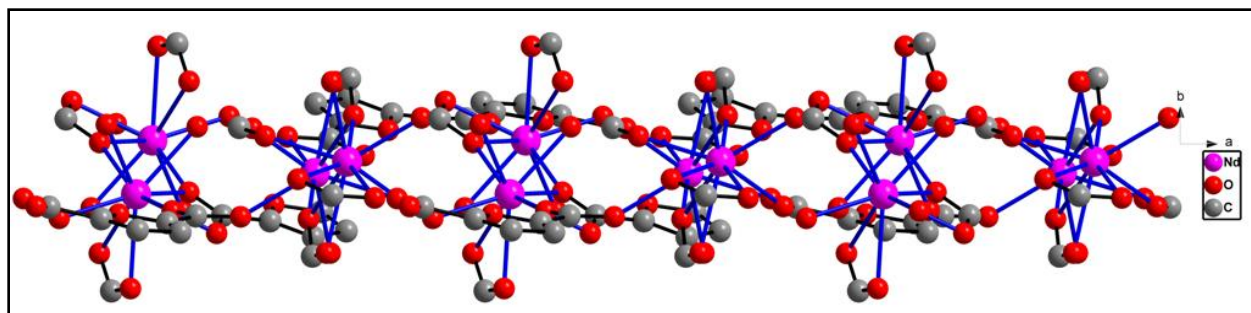


Fig. S17 Packing in CP **5** when view along c-axis.

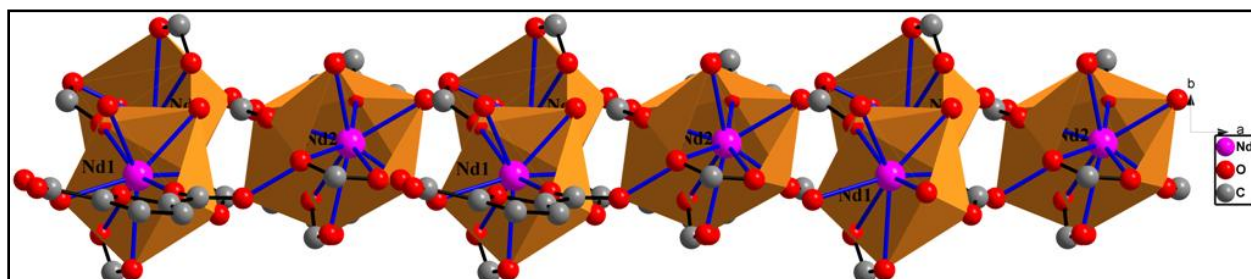


Fig. S18 Polyhedral packing arrangement of CP **5** when viewed along c-axis.

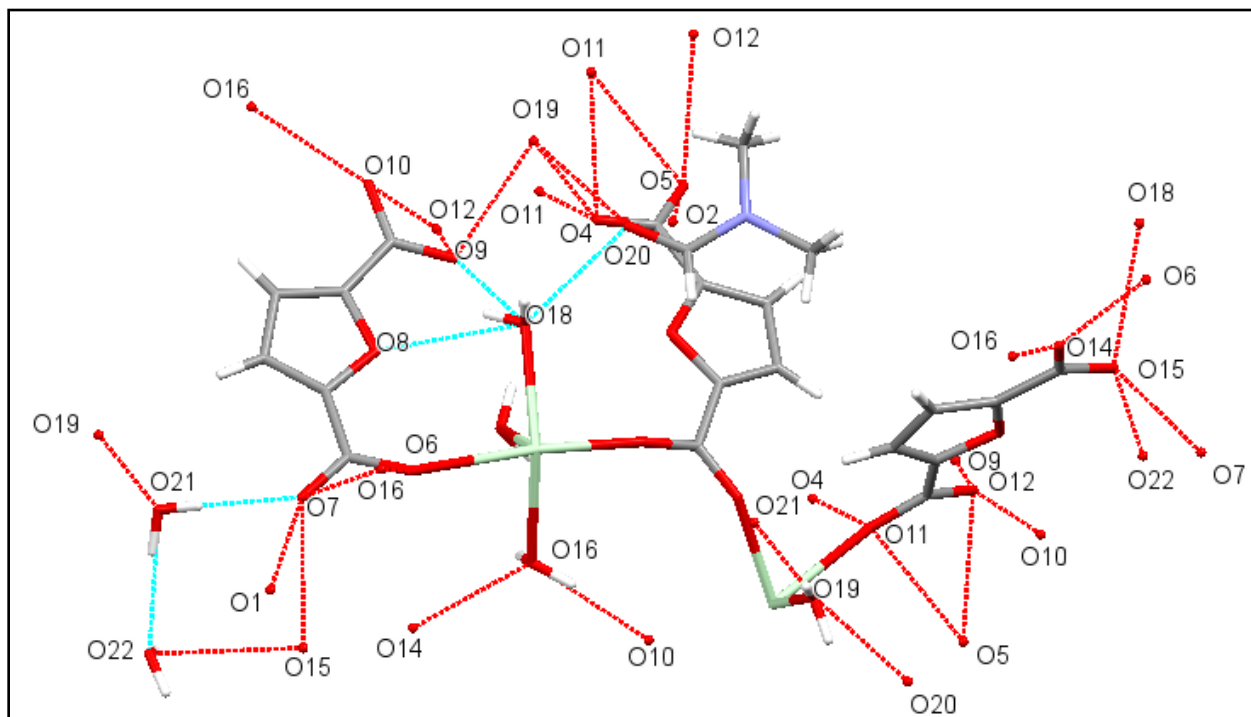


Fig. S19 Number and positions of Hydrogen bonds in asymmetric unit of CP **5**.

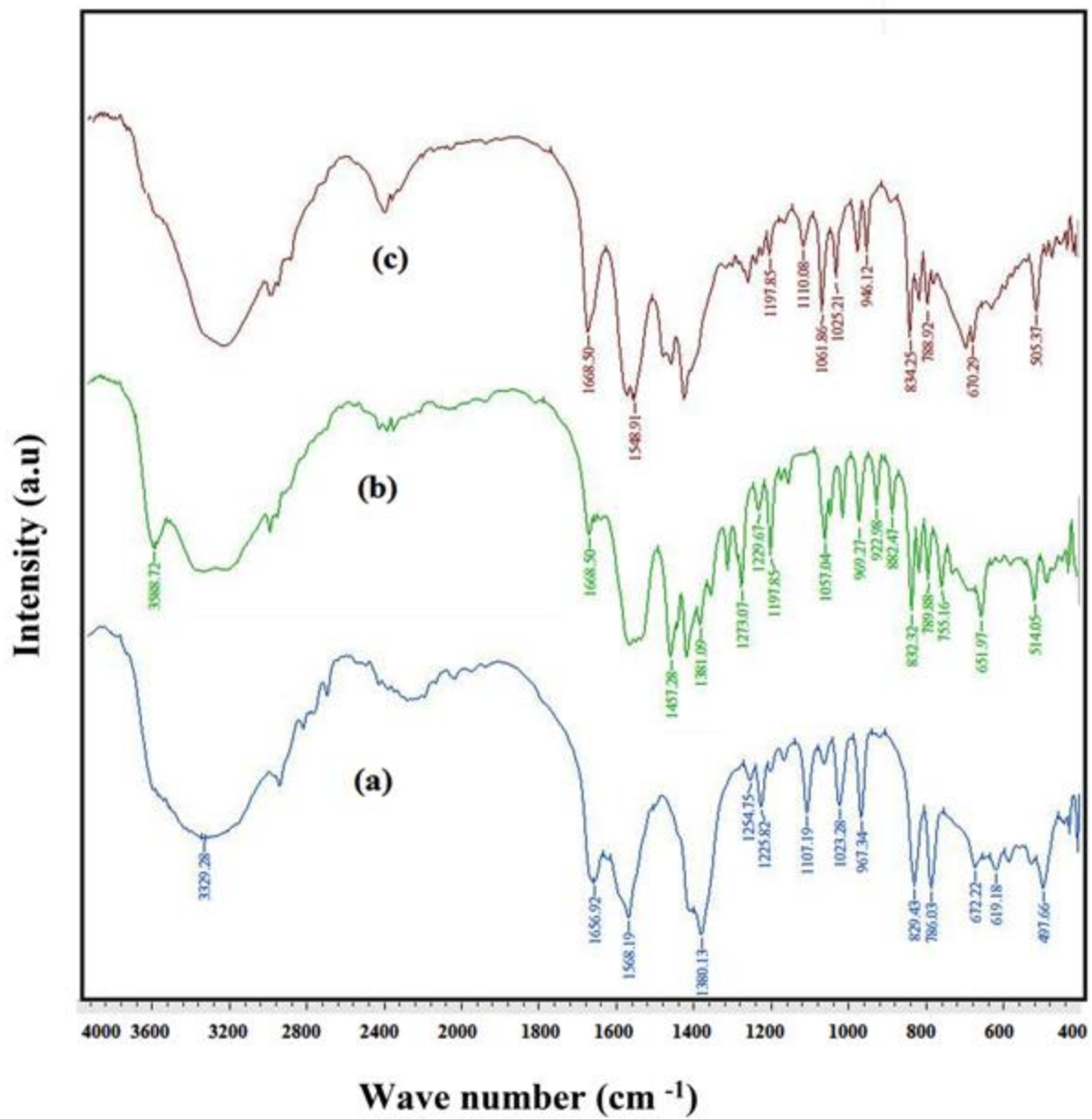


Fig. S20 FT-IR Spectra of CP 1-3; (a) CP 1, (b) CP 2 & (c) CP 3.

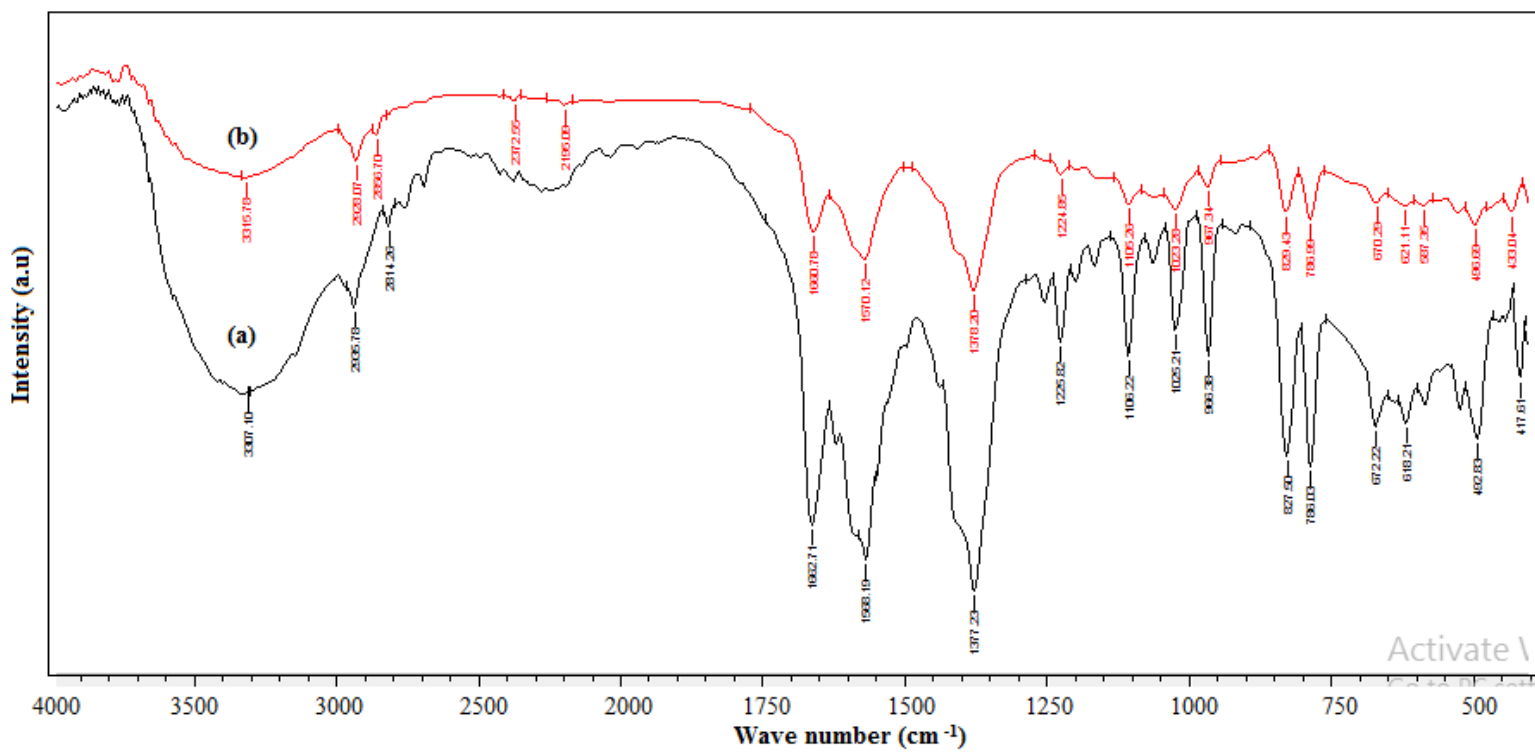


Fig. S21 FT-IR Spectra of CPs (a) CP 4 & (b) CP 5.

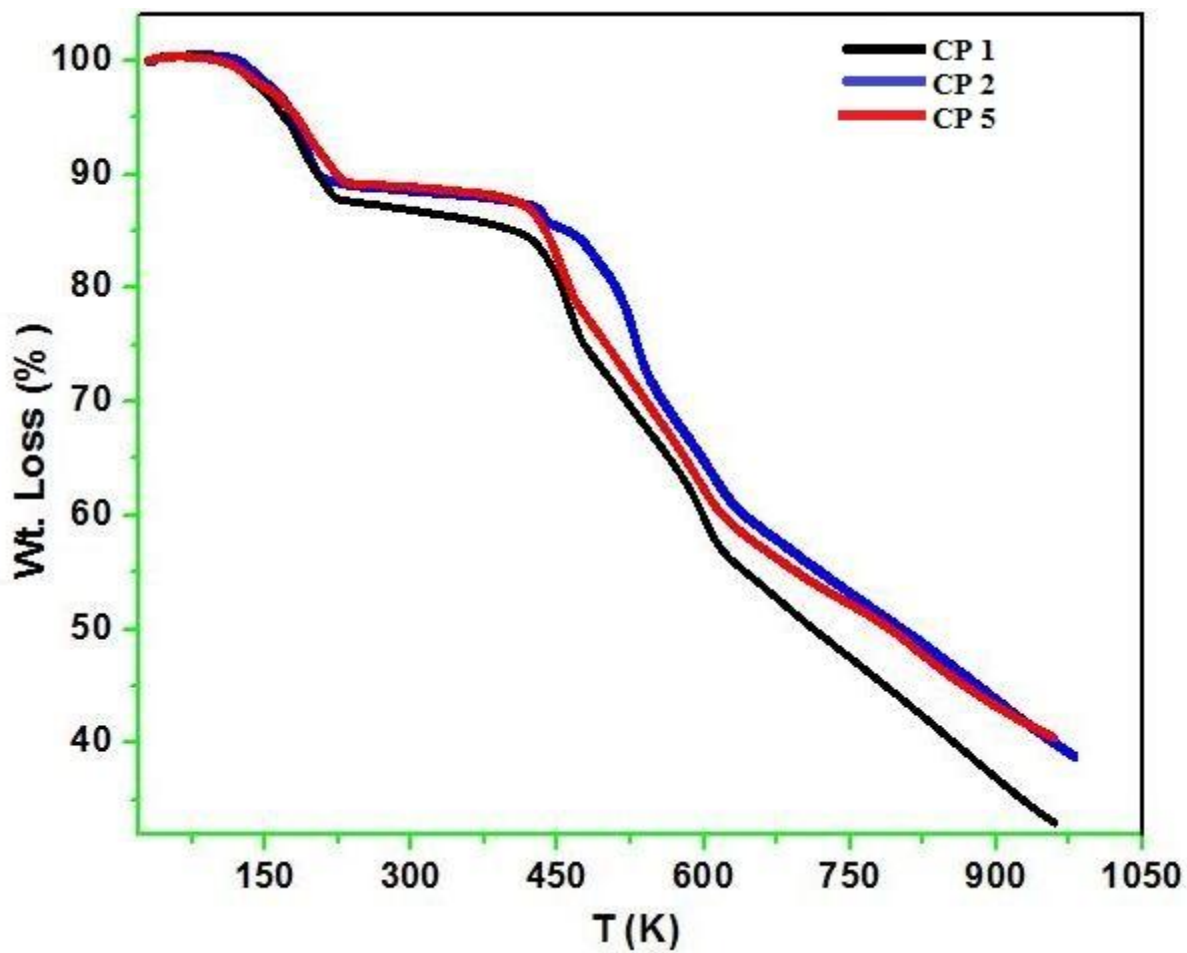


Fig. S22 TGA plots of CP 1 (black color), CP 2 (blue color) & CP 5 (red color).

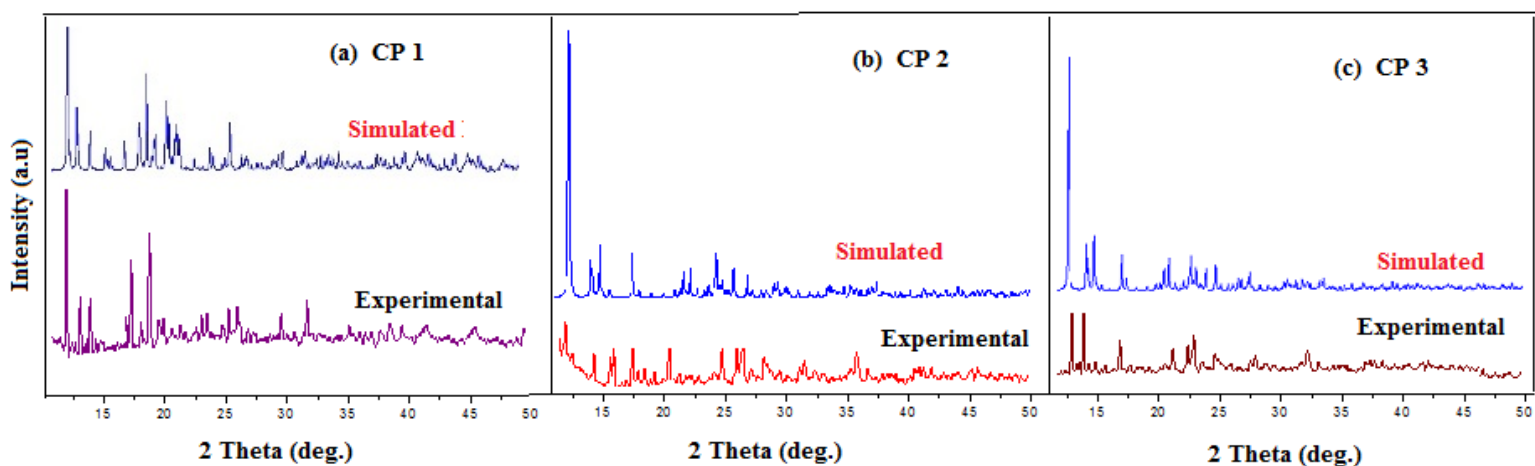


Fig.S23 Experimental and simulated powder X-ray diffraction pattern for CPs 1–3.

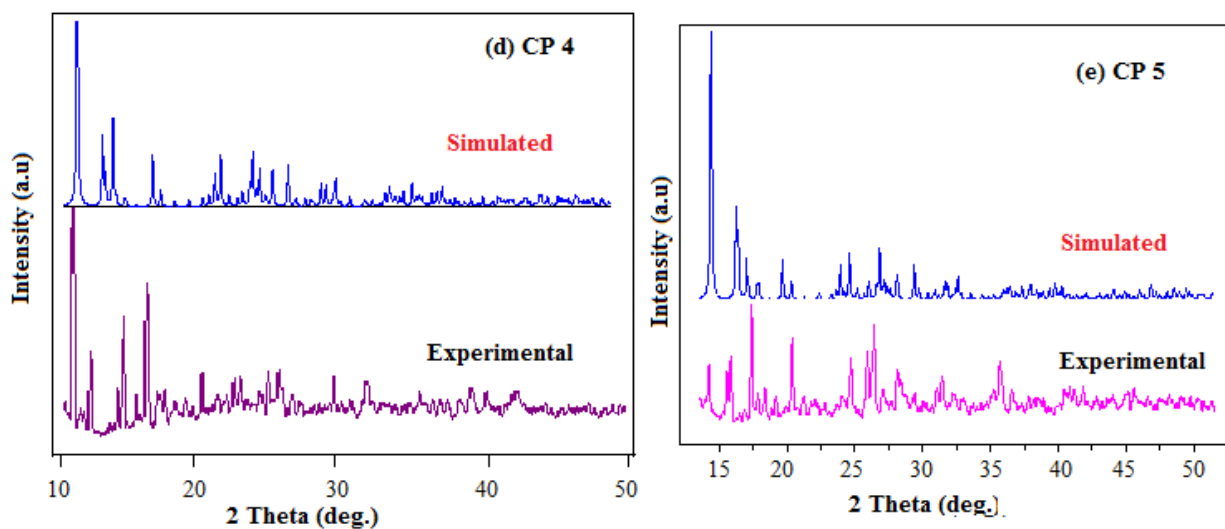


Fig. S24 Experimental and simulated powder X-ray diffraction pattern for CPs 4 & 5.

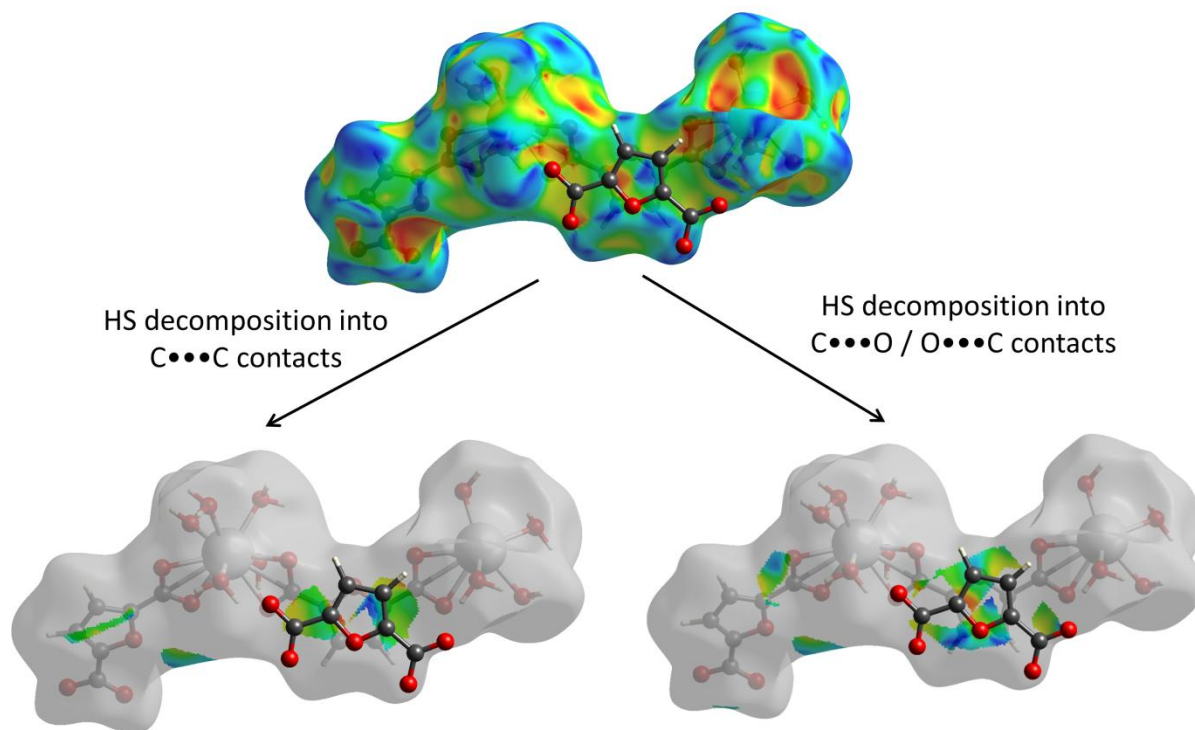


Fig. S25 Top: shape index-mapped HS generated for CP 1. Down: shape index-mapped contact-decomposed HSs generated for CP 1.

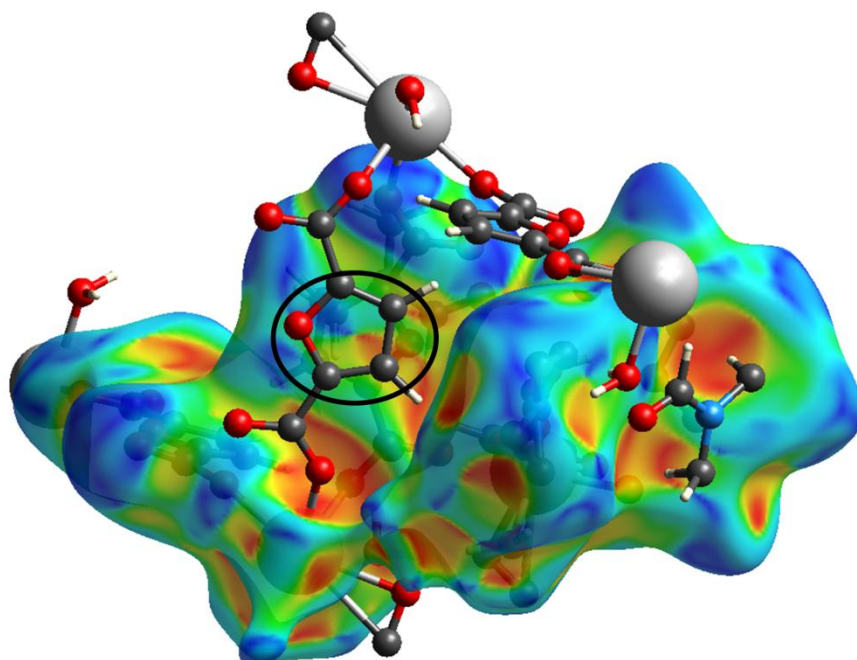


Fig. S26 Shape index-mapped HS generated for CP 1. (The region of heteroaromatic stacking is indicated with an oval)

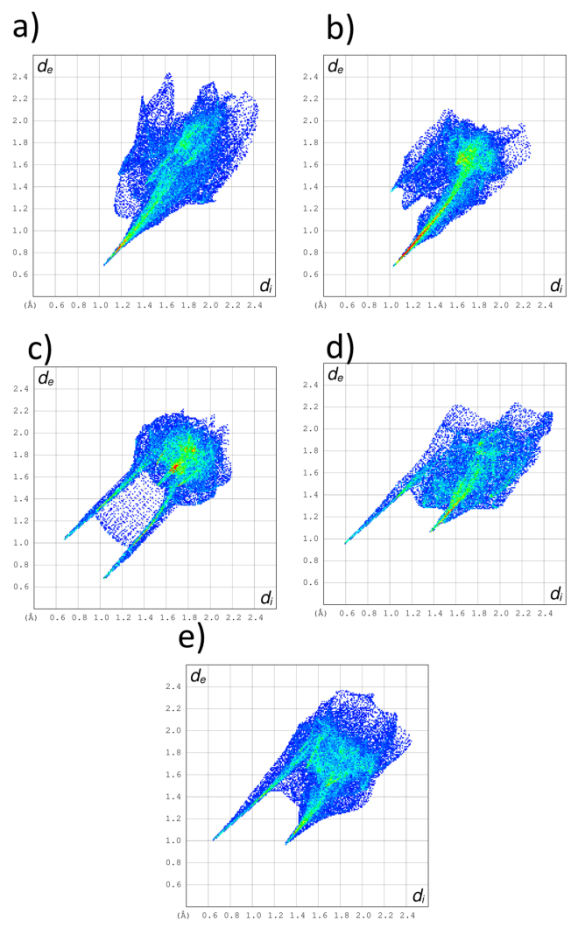


Fig. S27 2D fingerprint plots for (a)CP1, (b) YADGUH, (c) FURDCA, (d) UFALIZ, (e) UFALOF

Table S1
Selected Bond lengths (Å) for CP 1.

Pr1—O6	2.622 (2)	O9—C12	1.257 (4)
Pr1—O1	2.527 (2)	O21—H21A	0.825 (17)
Pr1—O7	2.514 (2)	O21—H21B	0.839 (17)
Pr1—O20	2.477 (3)	O23—H23A	0.824 (17)
Pr1—O2	2.594 (2)	O23—H23B	0.863 (18)
Pr1—O17	2.487 (2)	O13—C17	1.359 (4)
Pr1—O19	2.462 (2)	O13—C14	1.370 (4)
Pr1—O18	2.479 (3)	O18—H18A	0.847 (18)
Pr1—O16	2.504 (2)	O18—H18B	0.845 (18)
Pr1—C1	2.925 (3)	O16—H16A	0.835 (17)
Pr1—C7	2.938 (3)	O16—H16B	0.850 (17)
Pr2—O4	2.521 (2)	O27—H27A	0.8500
Pr2—O5	2.612 (2)	O27—H27B	0.8507
Pr2—O24	2.453 (2)	O31—H31A	0.8497
Pr2—H24A	2.6204	O31—H31B	0.8498
Pr2—O25	2.494 (2)	O14—C18	1.258 (4)
Pr2—O10 ⁱ	2.576 (2)	O11—C13	1.269 (4)
Pr2—O22	2.500 (2)	O15—C18	1.255 (4)
Pr2—O9 ⁱ	2.545 (2)	O26—H26A	0.8495
Pr2—O21	2.479 (2)	O26—H26B	0.8494
Pr2—O23	2.482 (2)	O28—H28A	0.8496

Pr2—C6	2.933 (3)	O28—H28B	0.8500
Pr2—C12 ⁱ	2.919 (3)	C6—C5	1.466 (4)
O6—C7	1.265 (4)	C1—C2	1.474 (4)
O4—C6	1.260 (4)	O29—H29A	0.8497
O3—C2	1.361 (4)	O29—H29B	0.8501
O3—C5	1.366 (3)	C2—C3	1.354 (4)
O5—C6	1.263 (4)	C5—C4	1.353 (4)
O24—H24A	0.8590	C7—C8	1.460 (5)
O24—H24B	0.8607	C12—C11	1.492 (4)
O25—H25A	0.816 (17)	C8—C9	1.345 (5)
O25—H25B	0.853 (17)	C17—C18	1.474 (5)
O1—C1	1.267 (3)	C17—C16	1.346 (5)
O10—C12	1.248 (4)	C14—C15	1.341 (5)
O8—C8	1.372 (4)	C14—C13	1.471 (5)
O8—C11	1.367 (4)	C11—C10	1.344 (4)
O7—C7	1.263 (4)	O12—C13	1.258 (4)
O20—H20A	0.826 (17)	C3—H3	0.9300
O20—H20B	0.851 (17)	C3—C4	1.420 (5)
O2—C1	1.253 (4)	C4—H4	0.9300
O17—H17A	0.812 (17)	C16—H16	0.9300
O17—H17B	0.828 (18)	C16—C15	1.414 (5)
O19—H19A	0.788 (17)	C9—H9	0.9300
O19—H19B	0.834 (17)	C9—C10	1.408 (5)

O22—H22A	0.844 (17)	C15—H15	0.9300
O22—H22B	0.832 (17)	C10—H10	0.9300

Symmetry code(s): (i) $x, y+1, z-1$.

Table S2
Selected Bond angles (°) for CP 1.

O6—Pr1—C1	132.80 (8)	O23—Pr2—C12 ⁱ	92.90 (10)
O6—Pr1—C7	25.49 (7)	C6—Pr2—H24A	95.4
O1—Pr1—O6	143.13 (8)	C12 ⁱ —Pr2—H24A	135.7
O1—Pr1—O2	50.83 (7)	C12 ⁱ —Pr2—C6	119.13 (9)
O1—Pr1—C1	25.56 (7)	C7—O6—Pr1	91.36 (19)
O1—Pr1—C7	140.46 (8)	C6—O4—Pr2	95.97 (18)
O7—Pr1—O6	50.72 (7)	C2—O3—C5	106.3 (2)
O7—Pr1—O1	124.90 (7)	C6—O5—Pr2	91.62 (18)
O7—Pr1—O2	74.44 (7)	Pr2—O24—H24A	91.5
O7—Pr1—C1	99.75 (8)	Pr2—O24—H24B	93.3
O7—Pr1—C7	25.28 (7)	H24A—O24—H24B	108.9
O20—Pr1—O6	69.26 (8)	Pr2—O25—H25A	127 (2)
O20—Pr1—O1	73.93 (8)	Pr2—O25—H25B	122 (2)
O20—Pr1—O7	85.59 (9)	H25A—O25—H25B	107 (3)
O20—Pr1—O2	72.87 (8)	C1—O1—Pr1	95.05 (19)
O20—Pr1—O17	126.66 (9)	C12—O10—Pr2 ⁱⁱ	92.91 (18)

O20—Pr1—O18	137.21 (8)	C11—O8—C8	106.2 (2)
O20—Pr1—O16	141.88 (8)	C7—O7—Pr1	96.48 (19)
O20—Pr1—C1	73.01 (8)	Pr1—O20—H20A	127 (2)
O20—Pr1—C7	77.38 (9)	Pr1—O20—H20B	125 (2)
O2—Pr1—O6	113.73 (7)	H20A—O20—H20B	106 (3)
O2—Pr1—C1	25.35 (8)	C1—O2—Pr1	92.25 (17)
O2—Pr1—C7	94.93 (8)	Pr1—O17—H17A	126 (2)
O17—Pr1—O6	133.79 (8)	Pr1—O17—H17B	122 (2)
O17—Pr1—O1	72.25 (8)	H17A—O17—H17B	105 (3)
O17—Pr1—O7	147.74 (9)	Pr1—O19—H19A	121 (2)
O17—Pr1—O2	112.48 (8)	Pr1—O19—H19B	114 (2)
O17—Pr1—O16	72.59 (8)	H19A—O19—H19B	119 (3)
O17—Pr1—C1	91.67 (9)	Pr2—O22—H22A	125 (2)
O17—Pr1—C7	147.19 (9)	Pr2—O22—H22B	126 (2)
O19—Pr1—O6	75.92 (8)	H22A—O22—H22B	100 (3)
O19—Pr1—O1	97.09 (8)	C12—O9—Pr2 ⁱⁱ	94.14 (19)
O19—Pr1—O7	126.63 (8)	Pr2—O21—H21A	126 (2)
O19—Pr1—O20	75.32 (9)	Pr2—O21—H21B	124 (2)
O19—Pr1—O2	139.88 (8)	H21A—O21—H21B	105 (3)
O19—Pr1—O17	69.42 (8)	Pr2—O23—H23A	130 (2)
O19—Pr1—O18	82.50 (9)	Pr2—O23—H23B	124 (2)
O19—Pr1—O16	139.43 (8)	H23A—O23—H23B	105 (3)
O19—Pr1—C1	120.27 (9)	C17—O13—C14	107.3 (3)

O19—Pr1—C7	101.36 (9)	Pr1—O18—H18A	127 (2)
O18—Pr1—O6	70.07 (8)	Pr1—O18—H18B	126 (2)
O18—Pr1—O1	145.91 (9)	H18A—O18—H18B	107 (3)
O18—Pr1—O7	78.94 (10)	Pr1—O16—H16A	128 (2)
O18—Pr1—O2	137.60 (8)	Pr1—O16—H16B	127 (2)
O18—Pr1—O17	75.85 (10)	H16A—O16—H16B	104 (3)
O18—Pr1—O16	74.89 (8)	H27A—O27—H27B	109.4
O18—Pr1—C1	148.70 (8)	H31A—O31—H31B	109.5
O18—Pr1—C7	71.69 (10)	H26A—O26—H26B	109.6
O16—Pr1—O6	124.57 (8)	H28A—O28—H28B	109.5
O16—Pr1—O1	84.32 (8)	O4—C6—Pr2	58.74 (16)
O16—Pr1—O7	81.69 (8)	O4—C6—O5	121.4 (3)
O16—Pr1—O2	69.13 (8)	O4—C6—C5	119.5 (3)
O16—Pr1—C1	73.99 (8)	O5—C6—Pr2	62.88 (17)
O16—Pr1—C7	102.81 (9)	O5—C6—C5	119.1 (3)
C1—Pr1—C7	118.84 (9)	C5—C6—Pr2	173.4 (2)
O4—Pr2—O5	50.72 (7)	O1—C1—Pr1	59.39 (16)
O4—Pr2—H24A	119.3	O1—C1—C2	118.8 (3)
O4—Pr2—O10 ⁱ	75.51 (7)	O2—C1—Pr1	62.40 (16)
O4—Pr2—O9 ⁱ	125.63 (7)	O2—C1—O1	121.5 (3)
O4—Pr2—C6	25.29 (7)	O2—C1—C2	119.7 (3)
O4—Pr2—C12 ⁱ	100.67 (8)	C2—C1—Pr1	172.7 (2)
O5—Pr2—H24A	72.1	H29A—O29—H29B	109.5

O5—Pr2—C6	25.50 (7)	O3—C2—C1	116.0 (3)
O5—Pr2—C12 ⁱ	131.87 (8)	C3—C2—O3	110.7 (3)
O24—Pr2—O4	125.25 (8)	C3—C2—C1	133.3 (3)
O24—Pr2—O5	74.57 (8)	O3—C5—C6	115.9 (3)
O24—Pr2—H24A	19.1	C4—C5—O3	110.3 (3)
O24—Pr2—O25	74.38 (9)	C4—C5—C6	133.8 (3)
O24—Pr2—O10 ⁱ	139.49 (9)	O6—C7—Pr1	63.15 (17)
O24—Pr2—O22	142.56 (8)	O6—C7—C8	119.6 (3)
O24—Pr2—O9 ⁱ	96.82 (8)	O7—C7—Pr1	58.23 (17)
O24—Pr2—O21	84.81 (9)	O7—C7—O6	121.2 (3)
O24—Pr2—O23	69.30 (9)	O7—C7—C8	119.2 (3)
O24—Pr2—C6	99.96 (9)	C8—C7—Pr1	173.1 (2)
O24—Pr2—C12 ⁱ	119.77 (10)	O10—C12—Pr2 ⁱⁱ	61.81 (16)
O25—Pr2—O4	87.19 (8)	O10—C12—O9	122.0 (3)
O25—Pr2—O5	69.92 (8)	O10—C12—C11	118.6 (3)
O25—Pr2—H24A	91.5	O9—C12—Pr2 ⁱⁱ	60.41 (16)
O25—Pr2—O10 ⁱ	72.42 (9)	O9—C12—C11	119.4 (3)
O25—Pr2—O22	140.14 (8)	C11—C12—Pr2 ⁱⁱ	174.2 (2)
O25—Pr2—O9 ⁱ	71.41 (8)	O8—C8—C7	116.3 (3)
O25—Pr2—C6	78.78 (9)	C9—C8—O8	109.4 (3)
O25—Pr2—C12 ⁱ	71.08 (9)	C9—C8—C7	134.2 (3)
O10 ⁱ —Pr2—O5	113.88 (7)	O13—C17—C18	114.6 (3)
O10 ⁱ —Pr2—H24A	158.2	C16—C17—O13	109.5 (3)

O10 ⁱ —Pr2—C6	95.71 (8)	C16—C17—C18	135.8 (3)
O10 ⁱ —Pr2—C12 ⁱ	25.28 (8)	O13—C14—C13	113.3 (3)
O22—Pr2—O4	79.59 (8)	C15—C14—O13	109.3 (3)
O22—Pr2—O5	123.73 (8)	C15—C14—C13	137.4 (3)
O22—Pr2—H24A	127.7	O8—C11—C12	115.5 (3)
O22—Pr2—O10 ⁱ	67.90 (8)	C10—C11—O8	110.5 (3)
O22—Pr2—O9 ⁱ	86.15 (8)	C10—C11—C12	133.8 (3)
O22—Pr2—C6	101.21 (9)	O14—C18—C17	117.4 (3)
O22—Pr2—C12 ⁱ	74.69 (8)	O15—C18—O14	124.9 (3)
O9 ⁱ —Pr2—O5	141.29 (8)	O15—C18—C17	117.8 (3)
O9 ⁱ —Pr2—H24A	110.9	C2—C3—H3	127.0
O9 ⁱ —Pr2—O10 ⁱ	50.67 (7)	C2—C3—C4	106.1 (3)
O9 ⁱ —Pr2—C6	140.19 (8)	C4—C3—H3	127.0
O9 ⁱ —Pr2—C12 ⁱ	25.44 (8)	C5—C4—C3	106.6 (3)
O21—Pr2—O4	77.43 (9)	C5—C4—H4	126.7
O21—Pr2—O5	71.85 (8)	C3—C4—H4	126.7
O21—Pr2—H24A	65.8	C17—C16—H16	126.6
O21—Pr2—O25	140.05 (8)	C17—C16—C15	106.8 (3)
O21—Pr2—O10 ⁱ	135.69 (8)	C15—C16—H16	126.6
O21—Pr2—O22	73.18 (8)	C8—C9—H9	126.2
O21—Pr2—O9 ⁱ	146.12 (8)	C8—C9—C10	107.7 (3)
O21—Pr2—O23	75.56 (10)	C10—C9—H9	126.2
O21—Pr2—C6	71.62 (9)	C14—C15—C16	107.1 (3)

O21—Pr2—C12 ⁱ	147.62 (9)	C14—C15—H15	126.5
O23—Pr2—O4	147.74 (8)	C16—C15—H15	126.5
O23—Pr2—O5	132.80 (9)	C11—C10—C9	106.2 (3)
O23—Pr2—H24A	63.7	C11—C10—H10	126.9
O23—Pr2—O25	125.01 (9)	C9—C10—H10	126.9
O23—Pr2—O10 ⁱ	113.30 (9)	O11—C13—C14	117.6 (3)
O23—Pr2—O22	75.98 (8)	O12—C13—O11	124.6 (4)
O23—Pr2—O9 ⁱ	73.51 (9)	O12—C13—C14	117.7 (3)
O23—Pr2—C6	146.30 (9)		

Symmetry code(s): (i) $x, y+1, z-1$; (ii) $x, y-1, z+1$.

Table S3
Number and positions of Hydrogen bonds [\AA and $^\circ$] of CP 1.

$D-H\cdots A$	$D-H$ (\AA)	$H\cdots A$ (\AA)	$D\cdots A$ (\AA)	$D-H\cdots A$ ($^\circ$)
O24—H24A \cdots O7 ⁱ	0.86	2.04	2.741 (3)	138.0
O24—H24B \cdots O30	0.86	2.12	2.750 (4)	129.5
O25—H25A \cdots O15 ⁱⁱ	0.816 (17)	2.07 (2)	2.803 (4)	148 (3)
O25—H25B \cdots O15	0.853 (17)	1.908 (18)	2.737 (4)	164 (3)
O20—H20A \cdots O11	0.826 (17)	1.970 (18)	2.789 (4)	170 (4)
O20—H20B \cdots O11 ⁱⁱⁱ	0.851 (17)	1.979 (18)	2.820 (4)	170 (3)
O17—H17A \cdots O26 ^{iv}	0.812 (17)	1.998 (19)	2.781 (4)	162 (3)
O17—H17B \cdots O1 ^{iv}	0.828 (18)	1.98 (2)	2.776 (3)	160 (4)
O19—H19A \cdots O27 ⁱⁱⁱ	0.788 (17)	2.031 (18)	2.819 (4)	178 (3)
O19—H19B \cdots O4 ^{iv}	0.834 (17)	1.943 (18)	2.768 (3)	170 (3)
O22—H22B \cdots O6 ^{iv}	0.832 (17)	1.911 (18)	2.735 (3)	171 (4)
O21—H21A \cdots O31	0.825 (17)	1.978 (19)	2.789 (4)	167 (3)
O21—H21B \cdots O2 ⁱ	0.839 (17)	1.869 (18)	2.703 (3)	172 (4)
O23—H23A \cdots O14 ^v	0.824 (17)	1.972 (18)	2.780 (4)	167 (3)
O23—H23B \cdots O9 ⁱ	0.863 (18)	1.914 (18)	2.774 (3)	174 (3)
O18—H18A \cdots O29 ⁱ	0.847 (18)	1.96 (2)	2.780 (4)	161 (4)
O18—H18B \cdots O10 ^{vi}	0.845 (18)	1.864 (18)	2.709 (3)	178 (4)
O16—H16A \cdots O28 ⁱ	0.835 (17)	2.011 (19)	2.834 (4)	168 (4)
O16—H16B \cdots O5 ⁱ	0.850 (17)	1.940 (18)	2.789 (3)	177 (3)
O27—H27A \cdots O31 ⁱ	0.85	1.93	2.779 (4)	175.3

O27—H27B···O12	0.85	1.86	2.708 (4)	176.2
O31—H31B···O12 ^v	0.85	2.01	2.859 (4)	175.3
O26—H26A···O11	0.85	1.97	2.739 (4)	149.1
O26—H26B···O27 ⁱⁱⁱ	0.85	1.95	2.780 (4)	166.2
O28—H28A···O14	0.85	1.92	2.765 (3)	171.2
O28—H28B···O26 ^{vii}	0.85	2.13	2.743 (4)	128.2
O29—H29A···O28	0.85	2.11	2.780 (4)	134.9
O29—H29B···O30	0.85	1.93	2.775 (5)	176.4

Symmetry code(s): (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y+1, -z$; (iii) $-x+2, -y, -z+1$; (iv) $-x+2, -y+1, -z+1$; (v) $x, y+1, z$; (vi) $-x+2, -y, -z+2$; (vii) $x-1, y, z$.

Table S4
Selected lengths (Å) for CP 2.

O19—C23	1.206 (7)	O1—C1	1.239 (7)
O19—C23A	1.212 (7)	O7—C7	1.250 (7)
O19—Pr2	2.419 (5)	O12—C13	1.251 (7)
N2—C23	1.357 (7)	O17—H17A	0.8746
N2—C24	1.462 (7)	O17—H17B	0.8755
N2—C25	1.460 (7)	O13—C14	1.357 (7)
C23—H23	0.9300	O13—C17	1.368 (7)
C24—H24A	0.9600	O9—C12	1.264 (8)
C24—H24B	0.9600	O15—C18	1.240 (7)
C24—H24C	0.9600	O8—C8	1.376 (8)
C25—H25A	0.9600	O8—C11	1.370 (8)
C25—H25B	0.9600	O14—C18	1.260 (8)
C25—H25C	0.9600	O16—H16A	0.86 (2)
N2A—C24A	1.464 (7)	O16—H16B	0.85 (2)
N2A—C25A	1.462 (7)	O18—H18A	0.8567
N2A—C23A	1.360 (7)	O18—H18B	0.8563
C24A—H24D	0.9600	O2—C1	1.235 (7)
C24A—H24E	0.9600	C13—C14	1.488 (8)

C24A—H24F	0.9600	C7—C8	1.474 (9)
C25A—H25D	0.9600	C6—C5	1.480 (8)
C25A—H25E	0.9600	C1—C2	1.479 (8)
C25A—H25F	0.9600	O22—H22A	0.8491
C23A—H23A	0.9300	O22—H22B	0.8503
O23—H23B	0.8497	C18—C17	1.478 (8)
O23—H23C	0.8500	C8—C9	1.338 (10)
Pr1—Pr1 ⁱ	4.0436 (6)	C12—C11	1.465 (9)
Pr1—O6 ⁱ	2.658 (5)	C14—C15	1.337 (9)
Pr1—O6	2.403 (4)	C4—H4	0.9300
Pr1—O4 ⁱⁱ	2.423 (4)	C4—C5	1.353 (9)
Pr1—O5 ⁱⁱⁱ	2.404 (4)	C4—C3	1.421 (9)
Pr1—O1	2.362 (4)	C2—C3	1.343 (9)
Pr1—O7 ⁱ	2.529 (5)	C15—H15	0.9300
Pr1—O15 ⁱⁱⁱ	2.643 (5)	C15—C16	1.411 (9)
Pr1—O14 ⁱⁱⁱ	2.488 (4)	C17—C16	1.345 (9)
Pr1—O16	2.427 (5)	C3—H3	0.9300
Pr1—C7 ⁱ	2.959 (6)	C16—H16	0.9300
Pr1—C18 ⁱⁱⁱ	2.921 (6)	C10—H10	0.9300
Pr2—O11 ^{iv}	2.849 (5)	C10—C9	1.418 (10)

Pr2—O11	2.370 (4)	C10—C11	1.352 (10)
Pr2—O10 ^v	2.579 (5)	C9—H9	0.9300
Pr2—O12 ^{iv}	2.526 (5)	O20—C22	1.213 (11)
Pr2—O17	2.463 (5)	N1—C22	1.354 (13)
Pr2—O9 ^v	2.490 (5)	N1—C19	1.449 (16)
Pr2—O18	2.415 (5)	N1—C20	1.415 (17)
Pr2—O2	2.257 (5)	C22—H22	0.9300
Pr2—C13 ^{iv}	3.049 (6)	C19—H19A	0.9600
Pr2—C12 ^v	2.889 (7)	C19—H19B	0.9600
O11—C13	1.260 (7)	C19—H19C	0.9600
O6—C7	1.268 (7)	C20—H20A	0.9600
O4—C6	1.260 (7)	C20—H20B	0.9600
O10—C12	1.252 (8)	C20—H20C	0.9600
O5—C6	1.250 (7)	O21—H21A	0.8501
O3—C2	1.364 (7)	O21—H21B	0.8501
O3—C5	1.363 (7)		

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

Table S5
Selected Bond angles(°) of CP 2.

C23—O19—Pr2	163.7 (9)	O9 ^v —Pr2—O10 ^v	51.42 (14)
C23A—O19—Pr2	135.1 (10)	O9 ^v —Pr2—O12 ^{iv}	83.65 (17)
C23—N2—C24	117.5 (15)	O9 ^v —Pr2—C13 ^{iv}	78.00 (17)
C23—N2—C25	119.1 (18)	O9 ^v —Pr2—C12 ^v	25.85 (17)
C25—N2—C24	119.6 (19)	O18—Pr2—O19	72.7 (2)
O19—C23—N2	121.9 (13)	O18—Pr2—O11 ^{iv}	144.46 (17)
O19—C23—H23	119.1	O18—Pr2—O10 ^v	70.35 (17)
N2—C23—H23	119.1	O18—Pr2—O12 ^{iv}	138.76 (17)
N2—C24—H24A	109.5	O18—Pr2—O17	142.90 (18)
N2—C24—H24B	109.5	O18—Pr2—O9 ^v	76.40 (18)
N2—C24—H24C	109.5	O18—Pr2—C13 ^{iv}	151.29 (18)
H24A—C24—H24B	109.5	O18—Pr2—C12 ^v	73.09 (19)
H24A—C24—H24C	109.5	O2—Pr2—O19	79.6 (2)
H24B—C24—H24C	109.5	O2—Pr2—O11 ^{iv}	122.32 (16)
N2—C25—H25A	109.5	O2—Pr2—O11	154.2 (2)
N2—C25—H25B	109.5	O2—Pr2—O10 ^v	78.4 (2)
N2—C25—H25C	109.5	O2—Pr2—O12 ^{iv}	77.98 (18)
H25A—C25—H25B	109.5	O2—Pr2—O17	81.08 (19)
H25A—C25—H25C	109.5	O2—Pr2—O9 ^v	129.9 (2)
H25B—C25—H25C	109.5	O2—Pr2—O18	87.65 (19)

C25A—N2A—C24A	116 (2)	O2—Pr2—C13 ^{iv}	99.02 (18)
C23A—N2A—C24A	123 (2)	O2—Pr2—C12 ^v	104.1 (2)
C23A—N2A—C25A	120 (2)	C12 ^v —Pr2—C13 ^{iv}	78.20 (18)
N2A—C24A—H24D	109.5	Pr2—O11—Pr2 ^{iv}	113.32 (16)
N2A—C24A—H24E	109.5	C13—O11—Pr2	158.3 (4)
N2A—C24A—H24F	109.5	C13—O11—Pr2 ^{iv}	86.7 (4)
H24D—C24A—H24E	109.5	Pr1—O6—Pr1 ⁱ	105.95 (16)
H24D—C24A—H24F	109.5	C7—O6—Pr1	156.2 (4)
H24E—C24A—H24F	109.5	C7—O6—Pr1 ⁱ	90.7 (4)
N2A—C25A—H25D	109.5	C6—O4—Pr1 ⁱⁱ	134.4 (4)
N2A—C25A—H25E	109.5	C12—O10—Pr2 ^{vi}	91.1 (4)
N2A—C25A—H25F	109.5	C6—O5—Pr1 ^{vii}	138.2 (4)
H25D—C25A—H25E	109.5	C5—O3—C2	106.4 (5)
H25D—C25A—H25F	109.5	C1—O1—Pr1	147.2 (4)
H25E—C25A—H25F	109.5	C7—O7—Pr1 ⁱ	97.2 (4)
O19—C23A—N2A	125.7 (16)	C13—O12—Pr2 ^{iv}	102.3 (4)
O19—C23A—H23A	117.2	Pr2—O17—H17A	110.8
N2A—C23A—H23A	117.2	Pr2—O17—H17B	110.4
H23B—O23—H23C	109.5	H17A—O17—H17B	108.2
O6—Pr1—Pr1 ⁱ	39.20 (11)	C14—O13—C17	106.4 (5)

O6 ⁱ —Pr1—Pr1 ⁱ	34.85 (9)	C12—O9—Pr2 ^{vi}	95.0 (4)
O6—Pr1—O6 ⁱ	74.05 (16)	C18—O15—Pr1 ^{vii}	90.1 (4)
O6—Pr1—O4 ⁱⁱ	76.74 (15)	C11—O8—C8	106.9 (5)
O6—Pr1—O5 ⁱⁱⁱ	75.78 (15)	C18—O14—Pr1 ^{vii}	97.0 (4)
O6—Pr1—O7 ⁱ	122.41 (15)	Pr1—O16—H16A	125 (5)
O6—Pr1—O15 ⁱⁱⁱ	157.88 (15)	Pr1—O16—H16B	131 (5)
O6—Pr1—O14 ⁱⁱⁱ	146.47 (15)	H16A—O16—H16B	104 (4)
O6—Pr1—O16	86.08 (18)	Pr2—O18—H18A	109.8
O6 ⁱ —Pr1—C7 ⁱ	25.37 (15)	Pr2—O18—H18B	109.5
O6—Pr1—C7 ⁱ	98.36 (16)	H18A—O18—H18B	109.1
O6 ⁱ —Pr1—C18 ⁱⁱⁱ	115.38 (16)	C1—O2—Pr2	176.7 (5)
O6—Pr1—C18 ⁱⁱⁱ	166.47 (17)	O11—C13—Pr2 ^{iv}	68.9 (3)
O4 ⁱⁱ —Pr1—Pr1 ⁱ	67.79 (10)	O11—C13—C14	119.8 (5)
O4 ⁱⁱ —Pr1—O6 ⁱ	68.43 (14)	O12—C13—Pr2 ^{iv}	54.0 (3)
O4 ⁱⁱ —Pr1—O7 ⁱ	71.23 (16)	O12—C13—O11	122.0 (6)
O4 ⁱⁱ —Pr1—O15 ⁱⁱⁱ	93.73 (15)	O12—C13—C14	118.2 (6)
O4 ⁱⁱ —Pr1—O14 ⁱⁱⁱ	134.88 (16)	C14—C13—Pr2 ^{iv}	165.7 (4)
O4 ⁱⁱ —Pr1—O16	141.22 (17)	O6—C7—Pr1 ⁱ	63.9 (3)
O4 ⁱⁱ —Pr1—C7 ⁱ	66.80 (16)	O6—C7—C8	118.3 (6)
O4 ⁱⁱ —Pr1—C18 ⁱⁱⁱ	115.23 (16)	O7—C7—Pr1 ⁱ	58.0 (3)

O5 ⁱⁱⁱ —Pr1—Pr1 ⁱ	67.39 (11)	O7—C7—O6	121.8 (6)
O5 ⁱⁱⁱ —Pr1—O6 ⁱ	68.73 (15)	O7—C7—C8	119.8 (6)
O5 ⁱⁱⁱ —Pr1—O4 ⁱⁱ	133.83 (15)	C8—C7—Pr1 ⁱ	177.0 (4)
O5 ⁱⁱⁱ —Pr1—O7 ⁱ	93.70 (17)	O4—C6—C5	114.7 (5)
O5 ⁱⁱⁱ —Pr1—O15 ⁱⁱⁱ	123.19 (14)	O5—C6—O4	127.2 (6)
O5 ⁱⁱⁱ —Pr1—O14 ⁱⁱⁱ	72.74 (15)	O5—C6—C5	118.1 (5)
O5 ⁱⁱⁱ —Pr1—O16	72.07 (17)	O1—C1—C2	118.0 (5)
O5 ⁱⁱⁱ —Pr1—C7 ⁱ	81.41 (17)	O2—C1—O1	125.3 (6)
O5 ⁱⁱⁱ —Pr1—C18 ⁱⁱⁱ	98.08 (17)	O2—C1—C2	116.6 (5)
O1—Pr1—Pr1 ⁱ	111.31 (11)	H22A—O22—H22B	109.5
O1—Pr1—O6	78.75 (15)	O15—C18—Pr1 ^{vii}	64.8 (3)
O1—Pr1—O6 ⁱ	136.83 (14)	O15—C18—O14	122.5 (6)
O1—Pr1—O4 ⁱⁱ	73.15 (16)	O15—C18—C17	120.1 (6)
O1—Pr1—O5 ⁱⁱⁱ	134.81 (17)	O14—C18—Pr1 ^{vii}	57.7 (3)
O1—Pr1—O7 ⁱ	131.49 (17)	O14—C18—C17	117.4 (5)
O1—Pr1—O15 ⁱⁱⁱ	79.38 (15)	C17—C18—Pr1 ^{vii}	175.1 (4)
O1—Pr1—O14 ⁱⁱⁱ	116.63 (16)	O8—C8—C7	116.5 (5)
O1—Pr1—O16	69.49 (16)	C9—C8—O8	109.4 (6)
O1—Pr1—C7 ⁱ	139.32 (16)	C9—C8—C7	134.1 (6)
O1—Pr1—C18 ⁱⁱⁱ	98.17 (16)	O10—C12—Pr2 ^{vi}	63.2 (4)

O7 ⁱ —Pr1—Pr1 ⁱ	84.10 (10)	O10—C12—O9	122.0 (6)
O7 ⁱ —Pr1—O6 ⁱ	50.13 (14)	O10—C12—C11	119.5 (6)
O7 ⁱ —Pr1—O15 ⁱⁱⁱ	71.28 (16)	O9—C12—Pr2 ^{vi}	59.2 (3)
O7 ⁱ —Pr1—C7 ⁱ	24.78 (15)	O9—C12—C11	118.5 (6)
O7 ⁱ —Pr1—C18 ⁱⁱⁱ	69.47 (16)	C11—C12—Pr2 ^{vi}	172.6 (5)
O15 ⁱⁱⁱ —Pr1—Pr1 ⁱ	153.23 (12)	O13—C14—C13	116.7 (5)
O15 ⁱⁱⁱ —Pr1—O6 ⁱ	121.38 (15)	C15—C14—O13	110.6 (5)
O15 ⁱⁱⁱ —Pr1—C7 ⁱ	96.00 (17)	C15—C14—C13	132.5 (6)
O15 ⁱⁱⁱ —Pr1—C18 ⁱⁱⁱ	25.11 (15)	C5—C4—H4	126.9
O14 ⁱⁱⁱ —Pr1—Pr1 ⁱ	131.19 (11)	C5—C4—C3	106.1 (6)
O14 ⁱⁱⁱ —Pr1—O6 ⁱ	104.37 (15)	C3—C4—H4	126.9
O14 ⁱⁱⁱ —Pr1—O7 ⁱ	71.36 (16)	O3—C2—C1	117.2 (5)
O14 ⁱⁱⁱ —Pr1—O15 ⁱⁱⁱ	50.46 (14)	C3—C2—O3	110.4 (5)
O14 ⁱⁱⁱ —Pr1—C7 ⁱ	88.17 (17)	C3—C2—C1	132.1 (6)
O14 ⁱⁱⁱ —Pr1—C18 ⁱⁱⁱ	25.35 (16)	C14—C15—H15	126.7
O16—Pr1—Pr1 ⁱ	117.20 (14)	C14—C15—C16	106.5 (6)
O16—Pr1—O6 ⁱ	139.23 (16)	C16—C15—H15	126.7
O16—Pr1—O7 ⁱ	144.73 (18)	O13—C17—C18	114.1 (5)
O16—Pr1—O15 ⁱⁱⁱ	89.41 (18)	C16—C17—O13	109.6 (5)
O16—Pr1—O14 ⁱⁱⁱ	73.59 (18)	C16—C17—C18	136.3 (6)

O16—Pr1—C7 ⁱ	151.19 (16)	O3—C5—C6	118.0 (5)
O16—Pr1—C18 ⁱⁱⁱ	80.53 (19)	C4—C5—O3	110.3 (5)
C7 ⁱ —Pr1—Pr1 ⁱ	59.50 (12)	C4—C5—C6	131.5 (6)
C18 ⁱⁱⁱ —Pr1—Pr1 ⁱ	149.27 (12)	C4—C3—H3	126.6
C18 ⁱⁱⁱ —Pr1—C7 ⁱ	92.52 (17)	C2—C3—C4	106.7 (6)
O19—Pr2—O11 ^{iv}	127.03 (19)	C2—C3—H3	126.6
O19—Pr2—O10 ^v	137.41 (19)	C15—C16—H16	126.6
O19—Pr2—O12 ^{iv}	139.54 (19)	C17—C16—C15	106.9 (6)
O19—Pr2—O17	70.55 (19)	C17—C16—H16	126.6
O19—Pr2—O9 ^v	135.85 (18)	C9—C10—H10	126.8
O19—Pr2—C13 ^{iv}	135.90 (19)	C11—C10—H10	126.8
O19—Pr2—C12 ^v	145.4 (2)	C11—C10—C9	106.4 (7)
O11—Pr2—O19	76.7 (2)	C8—C9—C10	107.7 (7)
O11—Pr2—O11 ^{iv}	66.68 (16)	C8—C9—H9	126.2
O11—Pr2—O10 ^v	126.65 (15)	C10—C9—H9	126.2
O11—Pr2—O12 ^{iv}	114.40 (15)	O8—C11—C12	117.5 (6)
O11—Pr2—O17	81.33 (16)	C10—C11—O8	109.7 (6)
O11—Pr2—O9 ^v	75.46 (15)	C10—C11—C12	132.7 (7)
O11—Pr2—O18	95.14 (17)	C22—N1—C19	117.9 (12)
O11 ^{iv} —Pr2—C13 ^{iv}	24.38 (14)	C22—N1—C20	120.3 (12)

O11—Pr2—C13 ^{iv}	90.81 (16)	C20—N1—C19	121.8 (13)
O11—Pr2—C12 ^v	101.30 (18)	O20—C22—N1	125.0 (10)
O11 ^{iv} —Pr2—C12 ^v	80.66 (16)	O20—C22—H22	117.5
O10 ^v —Pr2—O11 ^{iv}	95.52 (14)	N1—C22—H22	117.5
O10 ^v —Pr2—C13 ^{iv}	83.60 (16)	N1—C19—H19A	109.5
O10 ^v —Pr2—C12 ^v	25.67 (16)	N1—C19—H19B	109.5
O12 ^{iv} —Pr2—O11 ^{iv}	47.76 (13)	N1—C19—H19C	109.5
O12 ^{iv} —Pr2—O10 ^v	68.98 (16)	H19A—C19—H19B	109.5
O12 ^{iv} —Pr2—C13 ^{iv}	23.63 (15)	H19A—C19—H19C	109.5
O12 ^{iv} —Pr2—C12 ^v	73.34 (18)	H19B—C19—H19C	109.5
O17—Pr2—O11 ^{iv}	67.27 (15)	N1—C20—H20A	109.5
O17—Pr2—O10 ^v	139.66 (16)	N1—C20—H20B	109.5
O17—Pr2—O12 ^{iv}	72.98 (17)	N1—C20—H20C	109.5
O17—Pr2—O9 ^v	136.35 (16)	H20A—C20—H20B	109.5
O17—Pr2—C13 ^{iv}	65.77 (17)	H20A—C20—H20C	109.5
O17—Pr2—C12 ^v	143.95 (18)	H20B—C20—H20C	109.5
O9 ^v —Pr2—O11 ^{iv}	69.68 (15)	H21A—O21—H21B	109.5

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

Table S6
Number and positions of Hydrogen bonds [\AA and $^\circ$] in CP 2.

$D-H\cdots A$	$D-H$ (Å)	$H\cdots A$ (Å)	$D\cdots A$ (Å)	$D-H\cdots A$ (°)
C25 ^a H25A ^a O23 ¹	0.96	2.02	2.68	124.4
C23A ^b H23A ^b O17	0.93	2.25	2.862(19)	122.6
O17 H17A O9 ¹	0.87	1.91	2.720(6)	154.4
O17 H17B O15 ²	0.88	1.89	2.720(6)	158.7
O16 H16A O2 ²	0.86(2)	1.88(2)	2.726(9)	172(9)
O16 H16B O20 ²	0.85(2)	1.94(2)	2.783(8)	173(8)
O18 H18B O14	0.86	2.05	2.797(7)	144.8
O22 H22A O2 ¹	0.85	2.02	2.851(15)	165.8
O22 H22B O12 ³	0.85	2.02	2.827(8)	159.3
O21 H21A O2 ³	0.85	1.89	2.67(4)	152.3

¹1/2-X,1/2+Y,3/2-Z; ²-1+X,+Y,+Z; ³1-X,1-Y,2-Z

Table S7
Selected Bond lengths (Å) of CP 3.

Eu1—Eu1 ⁱ	4.3672 (4)	C18—C17	1.474 (7)
Eu1—O6 ⁱ	2.847 (3)	O21—H21D	0.8507
Eu1—O6	2.370 (3)	O21—H21E	0.8491
Eu1—O15 ⁱⁱ	2.494 (3)	C2—C1	1.477 (5)
Eu1—O7 ⁱ	2.529 (3)	C2—C3	1.351 (6)
Eu1—O17	2.459 (3)	C14—C15	1.335 (7)
Eu1—O14 ⁱⁱ	2.581 (3)	C12—C11	1.479 (5)
Eu1—O16	2.418 (3)	C8—C9	1.333 (6)
Eu1—H16B	2.8157	C5—C4	1.348 (6)
Eu1—O1	2.259 (3)	C4—H4	0.9300
Eu1—O19	2.418 (4)	C4—C3	1.411 (6)
Eu1—C7 ⁱ	3.046 (4)	C17—C16	1.353 (7)
Eu1—C18 ⁱⁱ	2.883 (5)	C10—H10	0.9300
Eu2—Eu2 ⁱⁱⁱ	4.0473 (4)	C10—C9	1.419 (6)
Eu2—O11	2.666 (3)	C10—C11	1.339 (6)
Eu2—O11 ⁱⁱⁱ	2.407 (3)	C3—H3	0.9300
Eu2—O4 ^{iv}	2.416 (3)	C9—H9	0.9300
Eu2—O5 ^v	2.400 (3)	N1—C22A	1.320 (16)

Eu2—O2	2.357 (3)	N1—C23	1.36 (2)
Eu2—O12	2.529 (3)	N1—C24	1.60 (2)
Eu2—O9 ^v	2.479 (3)	N1—C22	1.348 (11)
Eu2—O10 ^v	2.649 (3)	N1—C23A	1.350 (17)
Eu2—O18	2.435 (4)	N1—C24A	1.466 (12)
Eu2—C13	2.955 (4)	C15—H15	0.9300
Eu2—C12 ^v	2.923 (4)	C15—C16	1.417 (7)
O11—C13	1.264 (5)	C16—H16	0.9300
O6—C7	1.258 (5)	C19—H19	0.9300
O4—C6	1.253 (5)	C19—N2	1.320 (9)
O5—C6	1.255 (5)	N2—C21	1.442 (11)
O2—C1	1.243 (5)	N2—C20	1.431 (13)
O13—C14	1.375 (5)	O22—H22B	0.8499
O13—C17	1.365 (6)	O22—H22C	0.8503
O3—C2	1.362 (5)	C21—H21A	0.9600
O3—C5	1.368 (5)	C21—H21B	0.9600
O12—C13	1.244 (5)	C21—H21C	0.9600
O15—C18	1.260 (6)	C20—H20A	0.9600
O7—C7	1.253 (5)	C20—H20B	0.9600
O17—H17A	0.8509	C20—H20C	0.9600

O17—H17B	0.8495	C22A—H22A	0.9300
O14—C18	1.247 (5)	C23—H23A	0.9600
O8—C8	1.368 (5)	C23—H23B	0.9600
O8—C11	1.374 (5)	C23—H23C	0.9600
O9—C12	1.252 (5)	C24—H24A	0.9600
O16—H16A	0.8523	C24—H24B	0.9600
O16—H16B	0.8507	C24—H24C	0.9600
O10—C12	1.255 (5)	C22—H22	0.9300
O18—H18A	0.8526	C23A—H23D	0.9600
O18—H18B	0.8518	C23A—H23E	0.9600
O1—C1	1.235 (5)	C23A—H23F	0.9600
C13—C14	1.483 (6)	C24A—H24D	0.9600
C6—C5	1.484 (6)	C24A—H24E	0.9600
O19—C22A	1.228 (19)	C24A—H24F	0.9600
O19—C22	1.195 (9)	O23—H23G	0.8498
C7—C8	1.484 (6)	O23—H23H	0.8499
O20—C19	1.206 (8)		

Symmetry code(s): (i) $-x+1, -y+1, -z+1$; (ii) $-x+3/2, y+1/2, -z+3/2$; (iii) $-x+2, -y+1, -z+2$; (iv) $-x+1, -y+1, -z+2$; (v) $x+1, y, z$.

Table S8
Selected bond angles (°) for CP 3.

Eu1 ⁱ —Eu1—H16B	122.2	C7—O6—Eu1	158.3 (3)
O6 ⁱ —Eu1—Eu1 ⁱ	29.89 (6)	C6—O4—Eu2 ^{iv}	134.7 (3)
O6—Eu1—Eu1 ⁱ	36.76 (7)	C6—O5—Eu2 ^{vi}	138.0 (3)
O6—Eu1—O6 ⁱ	66.65 (11)	C1—O2—Eu2	147.1 (3)
O6—Eu1—O15 ⁱⁱ	75.46 (11)	C17—O13—C14	106.4 (3)
O6—Eu1—O7 ⁱ	114.46 (10)	C2—O3—C5	106.2 (3)
O6—Eu1—O17	81.57 (11)	C13—O12—Eu2	97.2 (3)
O6—Eu1—O14 ⁱⁱ	126.56 (11)	C18—O15—Eu1 ^{vii}	94.6 (3)
O6—Eu1—O16	94.63 (12)	C7—O7—Eu1 ⁱ	101.9 (3)
O6—Eu1—H16B	87.3	Eu1—O17—H17A	109.5
O6 ⁱ —Eu1—H16B	149.0	Eu1—O17—H17B	109.3
O6—Eu1—O19	76.74 (14)	H17A—O17—H17B	109.6
O6 ⁱ —Eu1—C7 ⁱ	24.35 (10)	C18—O14—Eu1 ^{vii}	90.8 (3)
O6—Eu1—C7 ⁱ	90.77 (11)	C8—O8—C11	106.2 (3)
O6—Eu1—C18 ⁱⁱ	101.27 (12)	C12—O9—Eu2 ^{vi}	97.8 (2)
O6 ⁱ —Eu1—C18 ⁱⁱ	80.65 (11)	Eu1—O16—H16A	109.7
O15 ⁱⁱ —Eu1—Eu1 ⁱ	68.71 (7)	Eu1—O16—H16B	109.2

O15 ⁱⁱ —Eu1—O6 ⁱ	69.64 (10)	H16A—O16—H16B	109.3
O15 ⁱⁱ —Eu1—O7 ⁱ	83.60 (12)	C12—O10—Eu2 ^{vi}	89.6 (3)
O15 ⁱⁱ —Eu1—O14 ⁱⁱ	51.35 (10)	Eu2—O18—H18A	109.5
O15 ⁱⁱ —Eu1—H16B	88.4	Eu2—O18—H18B	109.2
O15 ⁱⁱ —Eu1—C7 ⁱ	77.84 (12)	H18A—O18—H18B	109.3
O15 ⁱⁱ —Eu1—C18 ⁱⁱ	25.82 (12)	C1—O1—Eu1	177.8 (3)
O7 ⁱ —Eu1—Eu1 ⁱ	77.72 (7)	O11—C13—Eu2	64.5 (2)
O7 ⁱ —Eu1—O6 ⁱ	47.85 (9)	O11—C13—C14	117.7 (4)
O7 ⁱ —Eu1—O14 ⁱⁱ	68.98 (11)	O12—C13—Eu2	58.1 (2)
O7 ⁱ —Eu1—H16B	153.8	O12—C13—O11	122.5 (4)
O7 ⁱ —Eu1—C7 ⁱ	23.73 (11)	O12—C13—C14	119.8 (4)
O7 ⁱ —Eu1—C18 ⁱⁱ	73.29 (13)	C14—C13—Eu2	177.3 (3)
O17—Eu1—Eu1 ⁱ	70.58 (7)	O4—C6—O5	127.1 (4)
O17—Eu1—O6 ⁱ	67.17 (10)	O4—C6—C5	115.0 (4)
O17—Eu1—O15 ⁱⁱ	136.26 (11)	O5—C6—C5	117.9 (4)
O17—Eu1—O7 ⁱ	72.76 (12)	C22A—O19—Eu1	136.4 (7)
O17—Eu1—O14 ⁱⁱ	139.45 (11)	C22—O19—Eu1	165.0 (6)
O17—Eu1—H16B	127.4	O6—C7—Eu1 ⁱ	68.9 (2)
O17—Eu1—C7 ⁱ	65.66 (12)	O6—C7—C8	120.4 (4)
O17—Eu1—C18 ⁱⁱ	143.70 (12)	O7—C7—Eu1 ⁱ	54.3 (2)

O14 ⁱⁱ —Eu1—Eu1 ⁱ	112.73 (7)	O7—C7—O6	122.3 (4)
O14 ⁱⁱ —Eu1—O6 ⁱ	95.55 (10)	O7—C7—C8	117.2 (4)
O14 ⁱⁱ —Eu1—H16B	86.6	C8—C7—Eu1 ⁱ	164.8 (3)
O14 ⁱⁱ —Eu1—C7 ⁱ	83.57 (11)	O15—C18—Eu1 ^{vii}	59.6 (2)
O14 ⁱⁱ —Eu1—C18 ⁱⁱ	25.63 (11)	O15—C18—C17	117.7 (4)
O16—Eu1—Eu1 ⁱ	124.77 (9)	O14—C18—Eu1 ^{vii}	63.5 (2)
O16—Eu1—O6 ⁱ	143.86 (11)	O14—C18—O15	122.8 (4)
O16—Eu1—O15 ⁱⁱ	75.95 (12)	O14—C18—C17	119.5 (4)
O16—Eu1—O7 ⁱ	138.80 (12)	C17—C18—Eu1 ^{vii}	172.1 (3)
O16—Eu1—O17	143.41 (12)	H21D—O21—H21E	109.4
O16—Eu1—O14 ⁱⁱ	70.29 (11)	O3—C2—C1	117.3 (3)
O16—Eu1—H16B	16.6	C3—C2—O3	110.2 (4)
O16—Eu1—C7 ⁱ	150.92 (12)	C3—C2—C1	132.3 (4)
O16—Eu1—C18 ⁱⁱ	72.84 (12)	O13—C14—C13	115.9 (4)
O1—Eu1—Eu1 ⁱ	146.55 (9)	C15—C14—O13	110.0 (4)
O1—Eu1—O6 ⁱ	122.09 (11)	C15—C14—C13	134.1 (4)
O1—Eu1—O6	154.05 (15)	O9—C12—Eu2 ^{vi}	57.1 (2)
O1—Eu1—O15 ⁱⁱ	130.05 (14)	O9—C12—O10	122.1 (4)
O1—Eu1—O7 ⁱ	77.76 (12)	O9—C12—C11	118.5 (4)
O1—Eu1—O17	80.63 (13)	O10—C12—Eu2 ^{vi}	64.9 (2)

O1—Eu1—O14 ⁱⁱ	78.70 (14)	O10—C12—C11	119.4 (4)
O1—Eu1—O16	88.56 (13)	C11—C12—Eu2 ^{vi}	175.7 (3)
O1—Eu1—H16B	88.7	O8—C8—C7	115.8 (4)
O1—Eu1—O19	79.66 (15)	C9—C8—O8	110.5 (4)
O1—Eu1—C7 ⁱ	98.88 (12)	C9—C8—C7	133.6 (4)
O1—Eu1—C18 ⁱⁱ	104.27 (15)	O3—C5—C6	117.9 (4)
O19—Eu1—Eu1 ⁱ	105.57 (11)	C4—C5—O3	110.3 (4)
O19—Eu1—O6 ⁱ	127.06 (13)	C4—C5—C6	131.6 (4)
O19—Eu1—O15 ⁱⁱ	135.83 (13)	O2—C1—C2	117.9 (4)
O19—Eu1—O7 ⁱ	139.63 (13)	O1—C1—O2	125.1 (4)
O19—Eu1—O17	70.86 (13)	O1—C1—C2	117.0 (4)
O19—Eu1—O14 ⁱⁱ	137.34 (13)	C5—C4—H4	126.7
O19—Eu1—O16	72.85 (13)	C5—C4—C3	106.5 (4)
O19—Eu1—H16B	56.6	C3—C4—H4	126.7
O19—Eu1—C7 ⁱ	136.06 (13)	O13—C17—C18	117.4 (4)
O19—Eu1—C18 ⁱⁱ	145.33 (13)	C16—C17—O13	109.9 (4)
C7 ⁱ —Eu1—Eu1 ⁱ	54.08 (8)	C16—C17—C18	132.7 (5)
C7 ⁱ —Eu1—H16B	166.2	C9—C10—H10	126.4
C18 ⁱⁱ —Eu1—Eu1 ⁱ	90.01 (9)	C11—C10—H10	126.4
C18 ⁱⁱ —Eu1—H16B	88.8	C11—C10—C9	107.2 (4)

C18 ⁱⁱ —Eu1—C7 ⁱ	78.08 (12)	C2—C3—C4	106.7 (4)
O11—Eu2—Eu2 ⁱⁱⁱ	34.93 (6)	C2—C3—H3	126.6
O11 ⁱⁱⁱ —Eu2—Eu2 ⁱⁱⁱ	39.35 (8)	C4—C3—H3	126.6
O11 ⁱⁱⁱ —Eu2—O11	74.28 (11)	C8—C9—C10	106.4 (4)
O11 ⁱⁱⁱ —Eu2—O4 ^{iv}	76.66 (10)	C8—C9—H9	126.8
O11 ⁱⁱⁱ —Eu2—O12	122.45 (10)	C10—C9—H9	126.8
O11 ⁱⁱⁱ —Eu2—O9 ^v	146.46 (10)	O8—C11—C12	113.8 (4)
O11 ⁱⁱⁱ —Eu2—O10 ^v	157.65 (10)	C10—C11—O8	109.6 (4)
O11 ⁱⁱⁱ —Eu2—O18	85.71 (12)	C10—C11—C12	136.6 (4)
O11 ⁱⁱⁱ —Eu2—C13	98.53 (11)	C22A—N1—C23	125.9 (13)
O11—Eu2—C13	25.32 (10)	C22A—N1—C24	115.2 (13)
O11 ⁱⁱⁱ —Eu2—C12 ^v	166.28 (12)	C23—N1—C24	118.8 (13)
O11—Eu2—C12 ^v	115.15 (11)	C22—N1—C23A	122.4 (11)
O4 ^{iv} —Eu2—Eu2 ⁱⁱⁱ	67.57 (7)	C22—N1—C24A	117.3 (8)
O4 ^{iv} —Eu2—O11	68.23 (10)	C23A—N1—C24A	120.3 (12)
O4 ^{iv} —Eu2—O12	71.05 (11)	C14—C15—H15	126.4
O4 ^{iv} —Eu2—O9 ^v	134.94 (11)	C14—C15—C16	107.2 (4)
O4 ^{iv} —Eu2—O10 ^v	93.98 (10)	C16—C15—H15	126.4
O4 ^{iv} —Eu2—O18	141.17 (11)	C17—C16—C15	106.4 (4)
O4 ^{iv} —Eu2—C13	66.67 (11)	C17—C16—H16	126.8

O4 ^{iv} —Eu2—C12 ^v	115.58 (12)	C15—C16—H16	126.8
O5 ^v —Eu2—Eu2 ⁱⁱⁱ	67.32 (7)	O20—C19—H19	117.0
O5 ^v —Eu2—O11 ⁱⁱⁱ	75.79 (10)	O20—C19—N2	125.9 (7)
O5 ^v —Eu2—O11	68.67 (10)	N2—C19—H19	117.0
O5 ^v —Eu2—O4 ^{iv}	133.53 (11)	C19—N2—C21	120.4 (8)
O5 ^v —Eu2—O12	93.72 (12)	C19—N2—C20	119.8 (8)
O5 ^v —Eu2—O9 ^v	72.76 (11)	C20—N2—C21	119.7 (9)
O5 ^v —Eu2—O10 ^v	123.27 (10)	H22B—O22—H22C	109.5
O5 ^v —Eu2—O18	72.14 (12)	N2—C21—H21A	109.5
O5 ^v —Eu2—C13	81.34 (12)	N2—C21—H21B	109.5
O5 ^v —Eu2—C12 ^v	97.85 (12)	N2—C21—H21C	109.5
O2—Eu2—Eu2 ⁱⁱⁱ	111.35 (7)	H21A—C21—H21B	109.5
O2—Eu2—O11	136.84 (10)	H21A—C21—H21C	109.5
O2—Eu2—O11 ⁱⁱⁱ	78.71 (11)	H21B—C21—H21C	109.5
O2—Eu2—O4 ^{iv}	73.22 (11)	N2—C20—H20A	109.5
O2—Eu2—O5 ^v	134.99 (12)	N2—C20—H20B	109.5
O2—Eu2—O12	131.28 (12)	N2—C20—H20C	109.5
O2—Eu2—O9 ^v	116.69 (11)	H20A—C20—H20B	109.5
O2—Eu2—O10 ^v	79.15 (10)	H20A—C20—H20C	109.5
O2—Eu2—O18	69.50 (11)	H20B—C20—H20C	109.5

O2—Eu2—C13	139.21 (11)	O19—C22A—N1	123.8 (13)
O2—Eu2—C12 ^v	98.35 (11)	O19—C22A—H22A	118.1
O12—Eu2—Eu2 ⁱⁱⁱ	84.00 (7)	N1—C22A—H22A	118.1
O12—Eu2—O11	49.98 (9)	N1—C23—H23A	109.5
O12—Eu2—O10 ^v	71.53 (11)	N1—C23—H23B	109.5
O12—Eu2—C13	24.68 (11)	N1—C23—H23C	109.5
O12—Eu2—C12 ^v	69.53 (11)	H23A—C23—H23B	109.5
O9 ^v —Eu2—Eu2 ⁱⁱⁱ	131.13 (8)	H23A—C23—H23C	109.5
O9 ^v —Eu2—O11	104.23 (10)	H23B—C23—H23C	109.5
O9 ^v —Eu2—O12	71.44 (11)	N1—C24—H24A	109.5
O9 ^v —Eu2—O10 ^v	50.52 (10)	N1—C24—H24B	109.5
O9 ^v —Eu2—C13	88.08 (11)	N1—C24—H24C	109.5
O9 ^v —Eu2—C12 ^v	25.10 (11)	H24A—C24—H24B	109.5
O10 ^v —Eu2—Eu2 ⁱⁱⁱ	153.38 (8)	H24A—C24—H24C	109.5
O10 ^v —Eu2—O11	121.48 (10)	H24B—C24—H24C	109.5
O10 ^v —Eu2—C13	96.16 (12)	O19—C22—N1	124.3 (8)
O10 ^v —Eu2—C12 ^v	25.42 (11)	O19—C22—H22	117.9
O18—Eu2—Eu2 ⁱⁱⁱ	117.01 (9)	N1—C22—H22	117.9
O18—Eu2—O11	139.20 (11)	N1—C23A—H23D	109.5
O18—Eu2—O12	145.10 (11)	N1—C23A—H23E	109.5

O18—Eu2—O9 ^v	73.88 (12)	N1—C23A—H23F	109.5
O18—Eu2—O10 ^v	89.46 (12)	H23D—C23A—H23E	109.5
O18—Eu2—C13	151.28 (12)	H23D—C23A—H23F	109.5
O18—Eu2—C12 ^v	80.73 (13)	H23E—C23A—H23F	109.5
Eu2 ⁱⁱⁱ —O11—Eu2	105.72 (11)	H24D—C24A—H24E	109.5
C13—O11—Eu2	90.2 (3)	H24D—C24A—H24F	109.5
C13—O11—Eu2 ⁱⁱⁱ	156.7 (3)	H24E—C24A—H24F	109.5
Eu1—O6—Eu1 ⁱ	113.35 (11)	H23G—O23—H23H	109.5
C7—O6—Eu1 ⁱ	86.7 (2)		

Symmetry code(s): (i) $-x+1, -y+1, -z+1$; (ii) $-x+3/2, y+1/2, -z+3/2$; (iii) $-x+2, -y+1, -z+2$; (iv) $-x+1, -y+1, -z+2$; (v) $x+1, y, z$; (vi) $x-1, y, z$; (vii) $-x+3/2, y-1/2, -z+3/2$.

Table S9
Number and positions of Hydrogen bonds [\AA and $^\circ$] in CP 3.

$D-H\cdots A$	$D-H$ (\AA)	$H\cdots A$ (\AA)	$D\cdots A$ (\AA)	$D-H\cdots A$ ($^\circ$)
C23A ^b —H23F ^b —O23 ⁱ	0.96	1.77	2.66 (7)	153.6
O17—H17A—O10 ⁱⁱ	0.85	1.93	2.711 (5)	151.2
O17—H17B—O15 ⁱⁱⁱ	0.85	1.90	2.725 (5)	164.7
O16—H16A—O20 ^{iv}	0.85	2.01	2.785 (6)	150.6
O16—H16B—O9	0.85	2.02	2.796 (5)	150.8
O18—H18A—O21	0.85	2.07	2.725 (6)	133.2

O18—H18B...O20	0.85	1.99	2.777 (5)	152.6
O21—H21D...O7 ^y	0.85	2.00	2.817 (6)	161.9
O21—H21E...O22	0.85	2.06	2.856 (11)	156.9
O22—H22B...O23	0.85	3.00	3.64 (2)	134.8

Symmetry code(s): (i) $-x+3/2, y-1/2, -z+3/2$; (ii) $x+1, y, z$; (iii) $x-1/2, -y+1/2, z-1/2$; (iv) $x-1, y, z$; (v) $-x+1, -y+1, -z+1$.

Table S10
Selected Bond lengths (Å) of CP 4.

Ce01—O11	2.447 (3)	C1—C2	1.473 (6)
Ce01—O11 ⁱ	2.821 (3)	O20—C22	1.203 (9)
Ce01—O12 ⁱ	2.605 (4)	C18—C17	1.465 (7)
Ce01—O9 ⁱⁱ	2.569 (4)	C14—C15	1.337 (7)
Ce01—O10 ⁱⁱ	2.623 (4)	O21—H21G	0.8503
Ce01—O17	2.535 (4)	O21—H21H	0.8495
Ce01—O18	2.482 (4)	C2—C3	1.338 (7)
Ce01—O2	2.322 (4)	C17—C16	1.343 (7)
Ce01—C13 ⁱ	3.074 (5)	C11—C10	1.347 (8)
Ce01—O19	2.471 (4)	C5—C4	1.347 (7)
Ce01—C12 ⁱⁱ	2.950 (5)	C15—H15	0.9300
Ce02—Ce02 ⁱⁱⁱ	4.1326 (5)	C15—C16	1.416 (7)
Ce02—O6 ⁱⁱⁱ	2.707 (4)	C4—H4	0.9300
Ce02—O6	2.480 (3)	C4—C3	1.418 (7)
Ce02—O5 ^{iv}	2.476 (3)	C16—H16	0.9300
Ce02—O1	2.422 (3)	C10—H10	0.9300
Ce02—O14 ^v	2.550 (3)	C10—C9	1.426 (8)
Ce02—O7 ⁱⁱⁱ	2.592 (4)	C3—H3	0.9300
Ce02—O16	2.502 (4)	C9—H9	0.9300

Ce02—O4 ^v	2.458 (4)	N1—C21A	1.477 (13)
Ce02—O15 ^v	2.692 (4)	N1—C19A	1.328 (12)
Ce02—C7 ⁱⁱⁱ	3.008 (5)	N1—C20A	1.399 (17)
Ce02—C18 ^v	2.987 (5)	N1—C21	1.55 (3)
O11—C13	1.270 (6)	N1—C20	1.40 (3)
O6—C7	1.259 (6)	N1—C19	1.33 (2)
O5—C6	1.263 (6)	N2—C22	1.341 (11)
O12—C13	1.244 (6)	N2—C23	1.447 (13)
O9—C12	1.265 (6)	N2—C24	1.396 (14)
O1—C1	1.241 (5)	C22—H22	0.9300
O10—C12	1.254 (6)	O22—H22A	0.8501
O8—C8	1.375 (6)	O22—H22B	0.8496
O8—C11	1.369 (6)	C23—H23A	0.9600
O3—C2	1.372 (5)	C23—H23B	0.9600
O3—C5	1.372 (6)	C23—H23C	0.9600
O14—C18	1.255 (6)	C24—H24A	0.9600
O7—C7	1.249 (6)	C24—H24B	0.9600
O16—H16A	0.847 (19)	C24—H24C	0.9600
O16—H16B	0.851 (19)	C21A—H21A	0.9600
O4—C6	1.253 (6)	C21A—H21B	0.9600

O15—C18	1.254 (6)	C21A—H21C	0.9600
O13—C14	1.369 (6)	C19A—H19A	0.9300
O13—C17	1.389 (6)	C20A—H20A	0.9600
O17—H17A	0.8509	C20A—H20B	0.9600
O17—H17B	0.8496	C20A—H20C	0.9600
O18—H18A	0.8541	C21—H21D	0.9600
O18—H18B	0.8545	C21—H21E	0.9600
C7—C8	1.476 (7)	C21—H21F	0.9600
O2—C1	1.230 (6)	C20—H20D	0.9600
C13—C14	1.480 (7)	C20—H20E	0.9600
O19—C19A	1.199 (11)	C20—H20F	0.9600
O19—C19	1.22 (3)	C19—H19	0.9300
C8—C9	1.348 (8)	O23—H23D	0.8500
C6—C5	1.475 (7)	O23—H23E	0.8498
C12—C11	1.462 (7)		

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

Table S11
Selected Bond angles (°) of CP 4.

O11—Ce01—O11 ⁱ	67.15 (12)	Ce02—O16—H16B	128 (3)
O11—Ce01—O12 ⁱ	114.71 (11)	H16A—O16—H16B	103 (4)
O11—Ce01—O9 ⁱⁱ	74.78 (12)	C6—O4—Ce02 ^{vii}	139.4 (3)
O11—Ce01—O10 ⁱⁱ	125.01 (12)	C18—O15—Ce02 ^{vii}	90.9 (3)
O11—Ce01—O17	82.02 (12)	C14—O13—C17	106.6 (4)
O11—Ce01—O18	96.16 (13)	Ce01—O17—H17A	109.4
O11—Ce01—C13 ⁱ	91.23 (12)	Ce01—O17—H17B	109.2
O11 ⁱ —Ce01—C13 ⁱ	24.39 (11)	H17A—O17—H17B	109.5
O11—Ce01—O19	77.33 (15)	Ce01—O18—H18A	109.4
O11 ⁱ —Ce01—C12 ⁱⁱ	79.84 (12)	Ce01—O18—H18B	109.5
O11—Ce01—C12 ⁱⁱ	100.09 (14)	H18A—O18—H18B	109.3
O12 ⁱ —Ce01—O11 ⁱ	47.66 (10)	O6—C7—Ce02 ⁱⁱⁱ	64.1 (3)
O12 ⁱ —Ce01—O10 ⁱⁱ	69.06 (13)	O6—C7—C8	117.9 (5)
O12 ⁱ —Ce01—C13 ⁱ	23.50 (12)	O7—C7—Ce02 ⁱⁱⁱ	58.8 (3)
O12 ⁱ —Ce01—C12 ⁱⁱ	74.40 (14)	O7—C7—O6	122.8 (5)
O9 ⁱⁱ —Ce01—O11 ⁱ	70.16 (12)	O7—C7—C8	119.2 (5)
O9 ⁱⁱ —Ce01—O12 ⁱ	85.42 (13)	C8—C7—Ce02 ⁱⁱⁱ	177.1 (4)
O9 ⁱⁱ —Ce01—O10 ⁱⁱ	50.34 (11)	C1—O2—Ce01	175.4 (4)

O9 ⁱⁱ —Ce01—C13 ⁱ	79.19 (13)	O11—C13—Ce01 ⁱ	66.6 (3)
O9 ⁱⁱ —Ce01—C12 ⁱⁱ	25.31 (13)	O11—C13—C14	120.0 (4)
O10 ⁱⁱ —Ce01—O11 ⁱ	93.72 (11)	O12—C13—Ce01 ⁱ	56.6 (3)
O10 ⁱⁱ —Ce01—C13 ⁱ	82.62 (12)	O12—C13—O11	122.2 (4)
O10 ⁱⁱ —Ce01—C12 ⁱⁱ	25.14 (12)	O12—C13—C14	117.8 (4)
O17—Ce01—O11 ⁱ	67.36 (11)	C14—C13—Ce01 ⁱ	166.7 (4)
O17—Ce01—O12 ⁱ	71.85 (13)	C19A—O19—Ce01	164.7 (7)
O17—Ce01—O9 ⁱⁱ	136.82 (12)	C19—O19—Ce01	136.1 (12)
O17—Ce01—O10 ⁱⁱ	139.22 (13)	O8—C8—C7	116.6 (4)
O17—Ce01—C13 ⁱ	65.26 (13)	C9—C8—O8	109.5 (5)
O17—Ce01—C12 ⁱⁱ	143.52 (13)	C9—C8—C7	133.8 (5)
O18—Ce01—O11 ⁱ	145.07 (13)	O5—C6—C5	115.1 (5)
O18—Ce01—O12 ⁱ	138.26 (13)	O4—C6—O5	125.9 (5)
O18—Ce01—O9 ⁱⁱ	75.98 (14)	O4—C6—C5	118.9 (4)
O18—Ce01—O10 ⁱⁱ	70.31 (13)	O9—C12—Ce01 ^{vi}	60.2 (3)
O18—Ce01—O17	143.36 (14)	O9—C12—C11	118.0 (5)
O18—Ce01—C13 ⁱ	151.16 (14)	O10—C12—Ce01 ^{vi}	62.7 (3)
O18—Ce01—C12 ⁱⁱ	73.01 (14)	O10—C12—O9	122.5 (5)
O2—Ce01—O11	155.54 (16)	O10—C12—C11	119.5 (5)
O2—Ce01—O11 ⁱ	122.02 (12)	C11—C12—Ce01 ^{vi}	172.2 (4)

O2—Ce01—O12 ⁱ	77.06 (13)	O1—C1—C2	117.8 (4)
O2—Ce01—O9 ⁱⁱ	129.02 (16)	O2—C1—O1	125.1 (5)
O2—Ce01—O10 ⁱⁱⁱ	78.72 (16)	O2—C1—C2	117.1 (4)
O2—Ce01—O17	81.76 (15)	O14—C18—Ce02 ^{vii}	57.8 (3)
O2—Ce01—O18	86.15 (15)	O14—C18—C17	118.8 (4)
O2—Ce01—C13 ⁱ	98.43 (14)	O15—C18—Ce02 ^{vii}	64.3 (3)
O2—Ce01—O19	80.13 (18)	O15—C18—O14	122.0 (5)
O2—Ce01—C12 ⁱⁱ	103.85 (17)	O15—C18—C17	119.1 (5)
O19—Ce01—O11 ⁱ	127.72 (15)	C17—C18—Ce02 ^{vii}	176.5 (4)
O19—Ce01—O12 ⁱ	138.49 (15)	O13—C14—C13	116.9 (4)
O19—Ce01—O9 ⁱⁱ	135.25 (14)	C15—C14—O13	110.5 (4)
O19—Ce01—O10 ⁱⁱⁱ	138.51 (15)	C15—C14—C13	132.6 (5)
O19—Ce01—O17	70.89 (14)	H21G—O21—H21H	109.5
O19—Ce01—O18	73.02 (15)	O3—C2—C1	116.5 (4)
O19—Ce01—C13 ⁱ	135.81 (15)	C3—C2—O3	109.9 (4)
O19—Ce01—C12 ⁱⁱ	145.42 (15)	C3—C2—C1	133.3 (5)
C12 ⁱⁱ —Ce01—C13 ⁱ	78.26 (14)	O13—C17—C18	114.4 (4)
O6—Ce02—Ce02 ⁱⁱⁱ	39.13 (8)	C16—C17—O13	108.4 (4)
O6 ⁱⁱⁱ —Ce02—Ce02 ⁱⁱⁱ	35.31 (7)	C16—C17—C18	137.1 (5)
O6—Ce02—O6 ⁱⁱⁱ	74.45 (12)	O8—C11—C12	117.0 (5)

O6—Ce02—O14 ^v	146.88 (12)	C10—C11—O8	109.4 (5)
O6—Ce02—O7 ⁱⁱⁱ	121.57 (12)	C10—C11—C12	133.6 (5)
O6—Ce02—O16	86.59 (14)	O3—C5—C6	117.7 (4)
O6—Ce02—O15 ^v	158.58 (11)	C4—C5—O3	110.1 (4)
O6—Ce02—C7 ⁱⁱⁱ	98.03 (13)	C4—C5—C6	132.0 (5)
O6 ⁱⁱⁱ —Ce02—C7 ⁱⁱⁱ	24.73 (12)	C14—C15—H15	126.8
O6—Ce02—C18 ^v	166.62 (13)	C14—C15—C16	106.4 (5)
O6 ⁱⁱⁱ —Ce02—C18 ^v	114.42 (12)	C16—C15—H15	126.8
O5 ^{iv} —Ce02—Ce02 ⁱⁱⁱ	67.07 (8)	C5—C4—H4	126.8
O5 ^{iv} —Ce02—O6 ⁱⁱⁱ	68.14 (11)	C5—C4—C3	106.4 (5)
O5 ^{iv} —Ce02—O6	75.95 (12)	C3—C4—H4	126.8
O5 ^{iv} —Ce02—O14 ^v	135.09 (12)	C17—C16—C15	108.1 (5)
O5 ^{iv} —Ce02—O7 ⁱⁱⁱ	70.91 (13)	C17—C16—H16	125.9
O5 ^{iv} —Ce02—O16	141.72 (13)	C15—C16—H16	125.9
O5 ^{iv} —Ce02—O15 ^v	95.15 (12)	C11—C10—H10	126.4
O5 ^{iv} —Ce02—C7 ⁱⁱⁱ	66.56 (13)	C11—C10—C9	107.2 (5)
O5 ^{iv} —Ce02—C18 ^v	116.19 (13)	C9—C10—H10	126.4
O1—Ce02—Ce02 ⁱⁱⁱ	110.48 (9)	C2—C3—C4	107.3 (5)
O1—Ce02—O6 ⁱⁱⁱ	136.68 (11)	C2—C3—H3	126.4
O1—Ce02—O6	77.81 (12)	C4—C3—H3	126.4

O1—Ce02—O5 ^{iv}	73.28 (12)	C8—C9—C10	106.6 (5)
O1—Ce02—O14 ^v	117.46 (12)	C8—C9—H9	126.7
O1—Ce02—O7 ⁱⁱⁱ	132.08 (13)	C10—C9—H9	126.7
O1—Ce02—O16	69.82 (13)	C19A—N1—C21A	120.4 (9)
O1—Ce02—O4 ^v	133.87 (14)	C19A—N1—C20A	120.9 (9)
O1—Ce02—O15 ^v	80.98 (12)	C20A—N1—C21A	118.5 (10)
O1—Ce02—C7 ⁱⁱⁱ	139.32 (13)	C20—N1—C21	116.1 (15)
O1—Ce02—C18 ^v	99.66 (13)	C19—N1—C21	116.1 (17)
O14 ^v —Ce02—Ce02 ⁱⁱⁱ	131.18 (9)	C19—N1—C20	127.6 (17)
O14 ^v —Ce02—O6 ⁱⁱⁱ	103.77 (12)	C22—N2—C23	119.9 (10)
O14 ^v —Ce02—O7 ⁱⁱⁱ	71.75 (13)	C22—N2—C24	120.9 (10)
O14 ^v —Ce02—O15 ^v	49.42 (11)	C24—N2—C23	119.2 (11)
O14 ^v —Ce02—C7 ⁱⁱⁱ	88.14 (13)	O20—C22—N2	125.4 (8)
O14 ^v —Ce02—C18 ^v	24.61 (12)	O20—C22—H22	117.3
O7 ⁱⁱⁱ —Ce02—Ce02 ⁱⁱⁱ	83.38 (8)	N2—C22—H22	117.3
O7 ⁱⁱⁱ —Ce02—O6 ⁱⁱⁱ	49.04 (11)	H22A—O22—H22B	109.5
O7 ⁱⁱⁱ —Ce02—O15 ^v	71.74 (12)	N2—C23—H23A	109.5
O7 ⁱⁱⁱ —Ce02—C7 ⁱⁱⁱ	24.34 (12)	N2—C23—H23B	109.5
O7 ⁱⁱⁱ —Ce02—C18 ^v	69.91 (13)	N2—C23—H23C	109.5
O16—Ce02—Ce02 ⁱⁱⁱ	117.42 (12)	H23A—C23—H23B	109.5

O16—Ce02—O6 ⁱⁱⁱ	139.25 (13)	H23A—C23—H23C	109.5
O16—Ce02—O14 ^v	73.42 (14)	H23B—C23—H23C	109.5
O16—Ce02—O7 ⁱⁱⁱ	144.88 (14)	N2—C24—H24A	109.5
O16—Ce02—O15 ^v	88.92 (15)	N2—C24—H24B	109.5
O16—Ce02—C7 ⁱⁱⁱ	150.85 (13)	N2—C24—H24C	109.5
O16—Ce02—C18 ^v	80.25 (15)	H24A—C24—H24B	109.5
O4 ^v —Ce02—Ce02 ⁱⁱⁱ	66.83 (9)	H24A—C24—H24C	109.5
O4 ^v —Ce02—O6 ⁱⁱⁱ	68.53 (12)	H24B—C24—H24C	109.5
O4 ^v —Ce02—O6	75.16 (12)	N1—C21A—H21A	109.5
O4 ^v —Ce02—O5 ^{iv}	132.74 (12)	N1—C21A—H21B	109.5
O4 ^v —Ce02—O14 ^v	73.65 (12)	N1—C21A—H21C	109.5
O4 ^v —Ce02—O7 ⁱⁱⁱ	94.01 (14)	H21A—C21A—H21B	109.5
O4 ^v —Ce02—O16	71.90 (14)	H21A—C21A—H21C	109.5
O4 ^v —Ce02—O15 ^v	123.06 (11)	H21B—C21A—H21C	109.5
O4 ^v —Ce02—C7 ⁱⁱⁱ	81.45 (14)	O19—C19A—N1	125.2 (10)
O4 ^v —Ce02—C18 ^v	98.25 (13)	O19—C19A—H19A	117.4
O15 ^v —Ce02—Ce02 ⁱⁱⁱ	153.37 (9)	N1—C19A—H19A	117.4
O15 ^v —Ce02—O6 ⁱⁱⁱ	120.79 (12)	N1—C20A—H20A	109.5
O15 ^v —Ce02—C7 ⁱⁱⁱ	96.06 (13)	N1—C20A—H20B	109.5
O15 ^v —Ce02—C18 ^v	24.82 (12)	N1—C20A—H20C	109.5

C7 ⁱⁱⁱ —Ce02—Ce02 ⁱⁱⁱ	59.26 (10)	H20A—C20A—H20B	109.5
C18 ^v —Ce02—Ce02 ⁱⁱⁱ	148.71 (10)	H20A—C20A—H20C	109.5
C18 ^v —Ce02—C7 ⁱⁱⁱ	92.37 (14)	H20B—C20A—H20C	109.5
Ce01—O11—Ce01 ⁱ	112.85 (12)	N1—C21—H21D	109.5
C13—O11—Ce01 ⁱ	89.0 (3)	N1—C21—H21E	109.5
C13—O11—Ce01	156.2 (3)	N1—C21—H21F	109.5
Ce02—O6—Ce02 ⁱⁱⁱ	105.55 (12)	H21D—C21—H21E	109.5
C7—O6—Ce02 ⁱⁱⁱ	91.1 (3)	H21D—C21—H21F	109.5
C7—O6—Ce02	155.6 (3)	H21E—C21—H21F	109.5
C6—O5—Ce02 ^{iv}	135.7 (3)	N1—C20—H20D	109.5
C13—O12—Ce01 ⁱ	99.9 (3)	N1—C20—H20E	109.5
C12—O9—Ce01 ^{vi}	94.5 (3)	N1—C20—H20F	109.5
C1—O1—Ce02	146.9 (3)	H20D—C20—H20E	109.5
C12—O10—Ce01 ^{vi}	92.2 (3)	H20D—C20—H20F	109.5
C11—O8—C8	107.3 (4)	H20E—C20—H20F	109.5
C2—O3—C5	106.3 (4)	O19—C19—N1	123 (2)
C18—O14—Ce02 ^{vii}	97.6 (3)	O19—C19—H19	118.5
C7—O7—Ce02 ⁱⁱⁱ	96.8 (3)	N1—C19—H19	118.5
Ce02—O16—H16A	128 (3)	H23D—O23—H23E	109.5

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

Table S12
Number and positions of Hydrogen bonds [\AA and $^\circ$] in CP 4.

$D-H\cdots A$	$D-H$ (\AA)	$H\cdots A$ (\AA)	$D\cdots A$ (\AA)	$D-H\cdots A$ ($^\circ$)
$C20A^{a-H20B_a}\cdots O23$	0.96	1.88	2.72 (4)	145.6
$O16-H16A\cdots O21$	0.847 (19)	1.89 (2)	2.731 (7)	177 (4)
$O16-H16B\cdots O20^i$	0.851 (19)	1.91 (2)	2.761 (6)	175 (7)
$O17-H17A\cdots O15^i$	0.85	2.18	2.713 (5)	120.7
$O18-H18A\cdots O20$	0.85	1.99	2.788 (7)	155.4
$O21-H21G\cdots O22$	0.85	2.05	2.883 (14)	165.9
$O21-H21H\cdots O12^{ii}$	0.85	1.98	2.819 (6)	167.3
$O22-H22B\cdots O23^{iii}$	0.85	1.95	2.68 (3)	143.9

Symmetry code(s): (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z$; (iii) $-x+3/2, y-1/2, -z+1/2$.

Table S13
Selected Bond lengths (\AA) of CP 5.

$Nd1-O6$	2.413 (3)	$O16-H16B$	0.8716
$Nd1-O6^i$	2.818 (3)	$O18-H18A$	0.8743
$Nd1-O14^{ii}$	2.528 (4)	$O18-H18B$	0.8715

Nd1—O7 ⁱ	2.555 (3)	C13—C14	1.487 (7)
Nd1—O15 ⁱⁱ	2.578 (4)	O1—C1	1.221 (5)
Nd1—O16	2.496 (4)	C7—C8	1.466 (7)
Nd1—O18	2.452 (4)	C6—C5	1.482 (6)
Nd1—O1	2.291 (3)	C1—C2	1.484 (6)
Nd1—C7 ⁱ	3.056 (5)	C18—C17	1.463 (7)
Nd1—C18 ⁱⁱ	2.905 (5)	C12—C11	1.473 (6)
Nd1—O17	2.487 (5)	O21—H21D	0.8496
Nd2—Nd2 ⁱⁱⁱ	4.0746 (5)	O21—H21E	0.8505
Nd2—O11 ⁱⁱⁱ	2.666 (3)	C11—C10	1.339 (6)
Nd2—O11	2.443 (3)	O17—H17A	0.8762
Nd2—O5 ^{iv}	2.449 (3)	O17—H17B	0.9660
Nd2—O12 ⁱⁱⁱ	2.563 (4)	C8—C9	1.346 (7)
Nd2—O4 ^v	2.423 (3)	C14—C15	1.344 (8)
Nd2—O10 ^v	2.643 (3)	O20—C19	1.230 (9)
Nd2—O2	2.385 (3)	C2—C3	1.341 (7)
Nd2—O9 ^v	2.517 (3)	C4—H4	0.9300
Nd2—O19	2.468 (4)	C4—C3	1.413 (7)
Nd2—C13 ⁱⁱⁱ	2.972 (5)	C4—C5	1.359 (7)
Nd2—C12 ^v	2.947 (5)	C17—C16	1.339 (8)

O6—C7	1.269 (6)	C10—H10	0.9300
O11—C13	1.271 (6)	C10—C9	1.410 (7)
O5—C6	1.258 (6)	C9—H9	0.9300
O12—C13	1.239 (6)	C3—H3	0.9300
O14—C18	1.266 (6)	C15—H15	0.9300
O4—C6	1.253 (6)	C15—C16	1.408 (8)
O8—C11	1.383 (5)	C16—H16	0.9300
O8—C8	1.368 (5)	N1—C19	1.340 (11)
O7—C7	1.247 (6)	N1—C21	1.437 (14)
O15—C18	1.254 (6)	N1—C20	1.441 (13)
O10—C12	1.251 (6)	C19—H19	0.9300
O2—C1	1.240 (5)	O22—H22A	0.8505
O13—C14	1.377 (6)	O22—H22B	0.8499
O13—C17	1.374 (6)	C21—H21A	0.9600
O9—C12	1.259 (6)	C21—H21B	0.9600
O19—H19A	0.8723	C21—H21C	0.9600
O19—H19B	0.9180	C20—H20A	0.9600
O3—C2	1.361 (5)	C20—H20B	0.9600
O3—C5	1.369 (6)	C20—H20C	0.9600
O16—H16A	0.8726		

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

Table S14
Selected Bond angles (°) of CP 5.

O6—Nd1—O6 ⁱ	66.98 (12)	C12 ^v —Nd2—Nd2 ⁱⁱⁱ	149.08 (10)
O6—Nd1—O14 ⁱⁱ	75.59 (12)	C12 ^v —Nd2—C13 ⁱⁱⁱ	91.89 (13)
O6—Nd1—O7 ⁱ	114.83 (11)	Nd1—O6—Nd1 ⁱ	113.02 (12)
O6—Nd1—O15 ⁱⁱ	126.59 (12)	C7—O6—Nd1 ⁱ	88.3 (3)
O6—Nd1—O16	80.57 (12)	C7—O6—Nd1	157.0 (3)
O6—Nd1—O18	95.33 (13)	Nd2—O11—Nd2 ⁱⁱⁱ	105.71 (12)
O6—Nd1—C7 ⁱ	91.24 (12)	C13—O11—Nd2	155.9 (3)
O6 ⁱ —Nd1—C7 ⁱ	24.52 (11)	C13—O11—Nd2 ⁱⁱⁱ	90.9 (3)
O6—Nd1—C18 ⁱⁱ	101.33 (13)	C6—O5—Nd2 ^{iv}	134.0 (3)
O6 ⁱ —Nd1—C18 ⁱⁱ	80.90 (12)	C13—O12—Nd2 ⁱⁱⁱ	96.6 (3)
O6—Nd1—O17	78.36 (16)	C18—O14—Nd1 ^{vi}	94.0 (3)
O14 ⁱⁱ —Nd1—O6 ⁱ	69.87 (11)	C6—O4—Nd2 ^{vii}	139.1 (3)
O14 ⁱⁱ —Nd1—O7 ⁱ	84.61 (13)	C8—O8—C11	106.3 (3)
O14 ⁱⁱ —Nd1—O15 ⁱⁱ	51.24 (11)	C7—O7—Nd1 ⁱ	101.3 (3)
O14 ⁱⁱ —Nd1—C7 ⁱ	78.28 (13)	C18—O15—Nd1 ^{vi}	92.0 (3)
O14 ⁱⁱ —Nd1—C18 ⁱⁱ	25.76 (12)	C12—O10—Nd2 ^{vii}	91.2 (3)
O7 ⁱ —Nd1—O6 ⁱ	47.94 (10)	C1—O2—Nd2	148.6 (3)

O7 ⁱ —Nd1—O15 ⁱⁱ	69.57 (12)	C17—O13—C14	106.9 (4)
O7 ⁱ —Nd1—C7 ⁱ	23.59 (12)	C12—O9—Nd2 ^{vii}	96.9 (3)
O7 ⁱ —Nd1—C18 ⁱⁱ	74.42 (14)	Nd2—O19—H19A	95.2
O15 ⁱⁱ —Nd1—O6 ⁱ	95.42 (11)	Nd2—O19—H19B	151.3
O15 ⁱⁱ —Nd1—C7 ⁱ	83.49 (12)	H19A—O19—H19B	102.0
O15 ⁱⁱ —Nd1—C18 ⁱⁱ	25.55 (12)	C2—O3—C5	106.1 (4)
O16—Nd1—O6 ⁱ	67.90 (11)	Nd1—O16—H16A	110.8
O16—Nd1—O14 ⁱⁱ	136.91 (12)	Nd1—O16—H16B	110.3
O16—Nd1—O7 ⁱ	73.56 (13)	H16A—O16—H16B	108.3
O16—Nd1—O15 ⁱⁱ	141.00 (13)	Nd1—O18—H18A	110.3
O16—Nd1—C7 ⁱ	66.82 (13)	Nd1—O18—H18B	110.3
O16—Nd1—C18 ⁱⁱ	145.34 (14)	H18A—O18—H18B	108.4
O18—Nd1—O6 ⁱ	144.67 (13)	O11—C13—Nd2 ⁱⁱⁱ	63.7 (3)
O18—Nd1—O14 ⁱⁱ	76.30 (14)	O11—C13—C14	117.2 (4)
O18—Nd1—O7 ⁱ	138.91 (13)	O12—C13—Nd2 ⁱⁱⁱ	58.9 (3)
O18—Nd1—O15 ⁱⁱ	70.09 (13)	O12—C13—O11	122.4 (5)
O18—Nd1—O16	141.95 (14)	O12—C13—C14	120.4 (4)
O18—Nd1—C7 ⁱ	151.19 (15)	C14—C13—Nd2 ⁱⁱⁱ	176.7 (3)
O18—Nd1—C18 ⁱⁱ	72.69 (15)	C1—O1—Nd1	172.4 (4)
O18—Nd1—O17	71.64 (18)	O6—C7—Nd1 ⁱ	67.2 (2)

O1—Nd1—O6	154.98 (16)	O6—C7—C8	119.8 (4)
O1—Nd1—O6 ⁱ	122.23 (12)	O7—C7—Nd1 ⁱ	55.1 (2)
O1—Nd1—O14 ⁱⁱ	128.84 (16)	O7—C7—O6	121.6 (4)
O1—Nd1—O7 ⁱ	77.16 (13)	O7—C7—C8	118.6 (4)
O1—Nd1—O15 ⁱⁱ	77.60 (16)	C8—C7—Nd1 ⁱ	167.4 (3)
O1—Nd1—O16	82.34 (15)	O5—C6—C5	115.4 (4)
O1—Nd1—O18	87.00 (15)	O4—C6—O5	126.8 (4)
O1—Nd1—C7 ⁱ	98.66 (13)	O4—C6—C5	117.8 (4)
O1—Nd1—C18 ⁱⁱ	103.13 (17)	O2—C1—C2	118.1 (4)
O1—Nd1—O17	78.78 (18)	O1—C1—O2	125.7 (4)
C18 ⁱⁱ —Nd1—C7 ⁱ	78.52 (14)	O1—C1—C2	116.2 (4)
O17—Nd1—O6 ⁱ	128.97 (17)	O14—C18—Nd1 ^{vi}	60.2 (3)
O17—Nd1—O14 ⁱⁱ	136.10 (14)	O14—C18—C17	117.9 (5)
O17—Nd1—O7 ⁱ	138.82 (15)	O15—C18—Nd1 ^{vi}	62.5 (3)
O17—Nd1—O15 ⁱⁱ	135.60 (17)	O15—C18—O14	122.4 (5)
O17—Nd1—O16	70.48 (17)	O15—C18—C17	119.7 (5)
O17—Nd1—C7 ⁱ	137.15 (17)	C17—C18—Nd1 ^{vi}	173.1 (4)
O17—Nd1—C18 ⁱⁱ	144.12 (17)	O10—C12—Nd2 ^{vii}	63.7 (3)
O11 ⁱⁱⁱ —Nd2—Nd2 ⁱⁱⁱ	35.26 (7)	O10—C12—O9	121.7 (4)
O11—Nd2—Nd2 ⁱⁱⁱ	39.04 (8)	O10—C12—C11	119.6 (4)

O11—Nd2—O11 ⁱⁱⁱ	74.29 (12)	O9—C12—Nd2 ^{vii}	58.0 (2)
O11—Nd2—O5 ^{iv}	76.91 (11)	O9—C12—C11	118.7 (4)
O11—Nd2—O12 ⁱⁱⁱ	122.35 (11)	C11—C12—Nd2 ^{vii}	176.6 (3)
O11—Nd2—O10 ^v	157.81 (11)	H21D—O21—H21E	109.5
O11—Nd2—O9 ^v	147.04 (11)	O8—C11—C12	113.4 (4)
O11—Nd2—O19	86.77 (13)	C10—C11—O8	109.4 (4)
O11 ⁱⁱⁱ —Nd2—C13 ⁱⁱⁱ	25.32 (11)	C10—C11—C12	137.1 (5)
O11—Nd2—C13 ⁱⁱⁱ	98.49 (12)	Nd1—O17—H17A	96.8
O11 ⁱⁱⁱ —Nd2—C12 ^v	114.70 (12)	Nd1—O17—H17B	126.2
O11—Nd2—C12 ^v	167.11 (13)	H17A—O17—H17B	98.2
O5 ^{iv} —Nd2—Nd2 ⁱⁱⁱ	67.84 (8)	O8—C8—C7	116.8 (4)
O5 ^{iv} —Nd2—O11 ⁱⁱⁱ	68.35 (11)	C9—C8—O8	109.9 (4)
O5 ^{iv} —Nd2—O12 ⁱⁱⁱ	71.31 (13)	C9—C8—C7	133.3 (4)
O5 ^{iv} —Nd2—O10 ^v	93.20 (11)	O13—C14—C13	115.9 (4)
O5 ^{iv} —Nd2—O9 ^v	134.16 (12)	C15—C14—O13	109.3 (5)
O5 ^{iv} —Nd2—O19	141.76 (13)	C15—C14—C13	134.8 (5)
O5 ^{iv} —Nd2—C13 ⁱⁱⁱ	66.49 (13)	O3—C2—C1	116.6 (4)
O5 ^{iv} —Nd2—C12 ^v	114.52 (13)	C3—C2—O3	110.3 (4)
O12 ⁱⁱⁱ —Nd2—Nd2 ⁱⁱⁱ	84.14 (8)	C3—C2—C1	132.9 (4)
O12 ⁱⁱⁱ —Nd2—O11 ⁱⁱⁱ	49.72 (10)	C3—C4—H4	127.3

O12 ⁱⁱⁱ —Nd2—O10 ^v	71.18 (12)	C5—C4—H4	127.3
O12 ⁱⁱⁱ —Nd2—C13 ⁱⁱⁱ	24.46 (11)	C5—C4—C3	105.4 (5)
O12 ⁱⁱⁱ —Nd2—C12 ^v	68.91 (12)	O13—C17—C18	117.2 (4)
O4 ^v —Nd2—Nd2 ⁱⁱⁱ	67.04 (8)	C16—C17—O13	109.1 (5)
O4 ^v —Nd2—O11	74.85 (11)	C16—C17—C18	133.6 (5)
O4 ^v —Nd2—O11 ⁱⁱⁱ	69.10 (11)	C11—C10—H10	126.3
O4 ^v —Nd2—O5 ^{iv}	133.70 (12)	C11—C10—C9	107.4 (4)
O4 ^v —Nd2—O12 ⁱⁱⁱ	94.26 (13)	C9—C10—H10	126.3
O4 ^v —Nd2—O10 ^v	124.28 (11)	C8—C9—C10	106.9 (4)
O4 ^v —Nd2—O9 ^v	74.09 (11)	C8—C9—H9	126.5
O4 ^v —Nd2—O19	71.70 (13)	C10—C9—H9	126.5
O4 ^v —Nd2—C13 ⁱⁱⁱ	82.31 (13)	C2—C3—C4	107.7 (5)
O4 ^v —Nd2—C12 ^v	99.18 (13)	C2—C3—H3	126.2
O10 ^v —Nd2—Nd2 ⁱⁱⁱ	152.96 (9)	C4—C3—H3	126.2
O10 ^v —Nd2—O11 ⁱⁱⁱ	120.85 (11)	O3—C5—C6	117.6 (4)
O10 ^v —Nd2—C13 ⁱⁱⁱ	95.53 (13)	C4—C5—O3	110.6 (4)
O10 ^v —Nd2—C12 ^v	25.12 (12)	C4—C5—C6	131.6 (5)
O2—Nd2—Nd2 ⁱⁱⁱ	110.72 (8)	C14—C15—H15	126.5
O2—Nd2—O11 ⁱⁱⁱ	136.77 (11)	C14—C15—C16	106.9 (5)
O2—Nd2—O11	78.17 (12)	C16—C15—H15	126.5

O2—Nd2—O5 ^{iv}	73.42 (12)	C17—C16—C15	107.8 (5)
O2—Nd2—O12 ⁱⁱⁱ	132.36 (13)	C17—C16—H16	126.1
O2—Nd2—O4 ^v	133.37 (13)	C15—C16—H16	126.1
O2—Nd2—O10 ^v	79.97 (12)	C19—N1—C21	120.2 (10)
O2—Nd2—O9 ^v	116.79 (12)	C19—N1—C20	120.5 (10)
O2—Nd2—O19	69.46 (13)	C21—N1—C20	119.3 (11)
O2—Nd2—C13 ⁱⁱⁱ	139.36 (13)	O20—C19—N1	126.1 (9)
O2—Nd2—C12 ^v	98.85 (13)	O20—C19—H19	116.9
O9 ^v —Nd2—Nd2 ⁱⁱⁱ	131.63 (8)	N1—C19—H19	116.9
O9 ^v —Nd2—O11 ⁱⁱⁱ	104.27 (11)	H22A—O22—H22B	109.5
O9 ^v —Nd2—O12 ⁱⁱⁱ	70.93 (12)	N1—C21—H21A	109.5
O9 ^v —Nd2—O10 ^v	50.21 (10)	N1—C21—H21B	109.5
O9 ^v —Nd2—C13 ⁱⁱⁱ	88.06 (13)	N1—C21—H21C	109.5
O9 ^v —Nd2—C12 ^v	25.09 (12)	H21A—C21—H21B	109.5
O19—Nd2—Nd2 ⁱⁱⁱ	117.70 (11)	H21A—C21—H21C	109.5
O19—Nd2—O11 ⁱⁱⁱ	139.65 (12)	H21B—C21—H21C	109.5
O19—Nd2—O12 ⁱⁱⁱ	143.93 (13)	N1—C20—H20A	109.5
O19—Nd2—O10 ^v	89.20 (14)	N1—C20—H20B	109.5
O19—Nd2—O9 ^v	73.26 (14)	N1—C20—H20C	109.5
O19—Nd2—C13 ⁱⁱⁱ	151.18 (13)	H20A—C20—H20B	109.5

O19—Nd2—C12 ^v	80.48 (14)	H20A—C20—H20C	109.5
C13 ⁱⁱⁱ —Nd2—Nd2 ⁱⁱⁱ	59.81 (9)	H20B—C20—H20C	109.5

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

Table S15

Number and positions of Hydrogen bonds [\AA and $^\circ$] in CP 5.

$D-H\cdots A$	$D-H$ (\AA)	$H\cdots A$ (\AA)	$D\cdots A$ (\AA)	$D-H\cdots A$ ($^\circ$)
O19—H19A \cdots O20 ⁱ	0.87	2.13	2.760 (6)	128.1
O19—H19B \cdots O21 ⁱⁱ	0.92	1.95	2.723 (7)	141.0
O16—H16A \cdots O10 ⁱ	0.87	1.91	2.746 (5)	160.2
O18—H18B \cdots O9	0.87	2.05	2.770 (5)	139.6
O21—H21D \cdots O22	0.85	2.01	2.847 (13)	170.9
O21—H21E \cdots O7	0.85	2.01	2.810 (6)	156.5

Symmetry code(s): (i) $x+1, y, z$; (ii) $-x+1, -y+1, -z+1$.

Table S 16

Contact contributions calculated for 2,5-FDA²⁻ in 1 and reference structures taken from the literature (CSD ref. codes: YADGUH, FURDCA, UFALIZ, UFALOF)

Compound / CSD refcode	2,5-FDA ²⁻		H ₂ -2,5-FDA		
	1	YADGUH	FURDCA	UFALIZ	UFALOF
O \cdots H/ H \cdots O	56.1	59.2	54.2	50.9	51.7
H \cdots H	17.5	15.1	8.0	23.9	16.1

C...H/ H...C	9.4	7.7	9.9	15.6	14.2
C...C	5.1	8.7	4.8	0.6	2.0
C...O/ O...C	6.8	6.8	13	4.7	9.8
O...O	8.4	2.5	10.1	3.0	4.7