

SUPPLEMENTARY MATERIAL

Diverse Coordination Numbers and Geometries in Pyridyl Adducts of Lanthanide(III) Complexes Based on β -Diketonate

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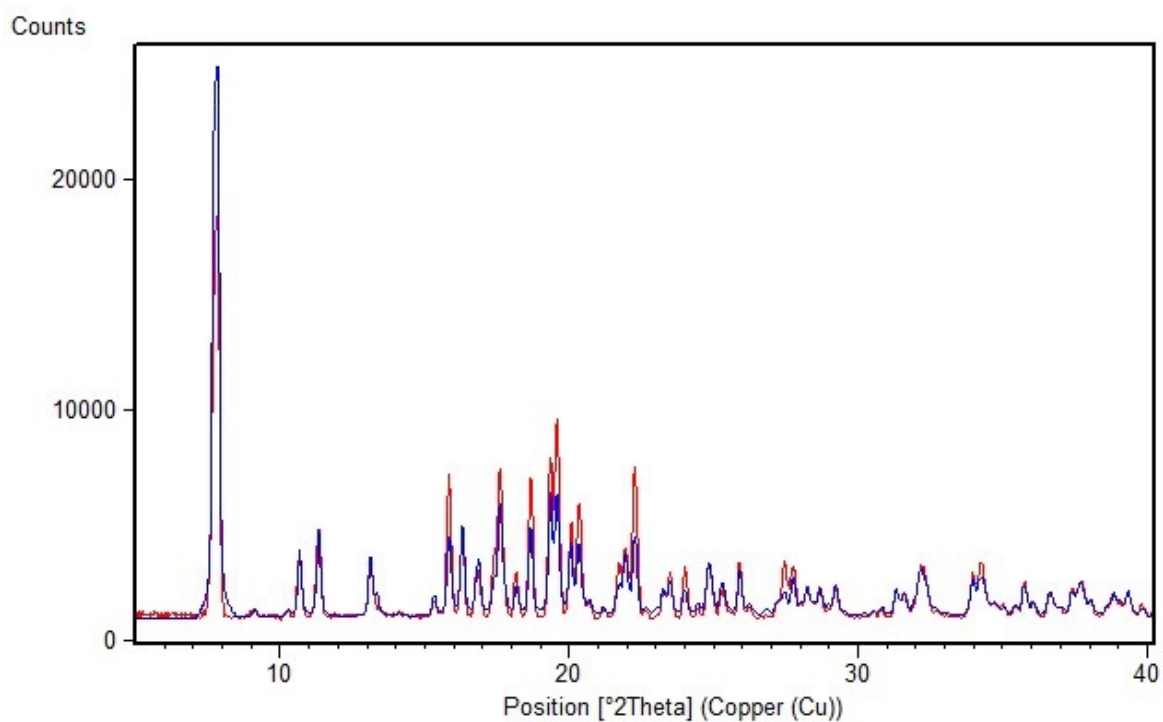


Figure S1: X-ray powder pattern of **1** (red: observed, blue: simulated).

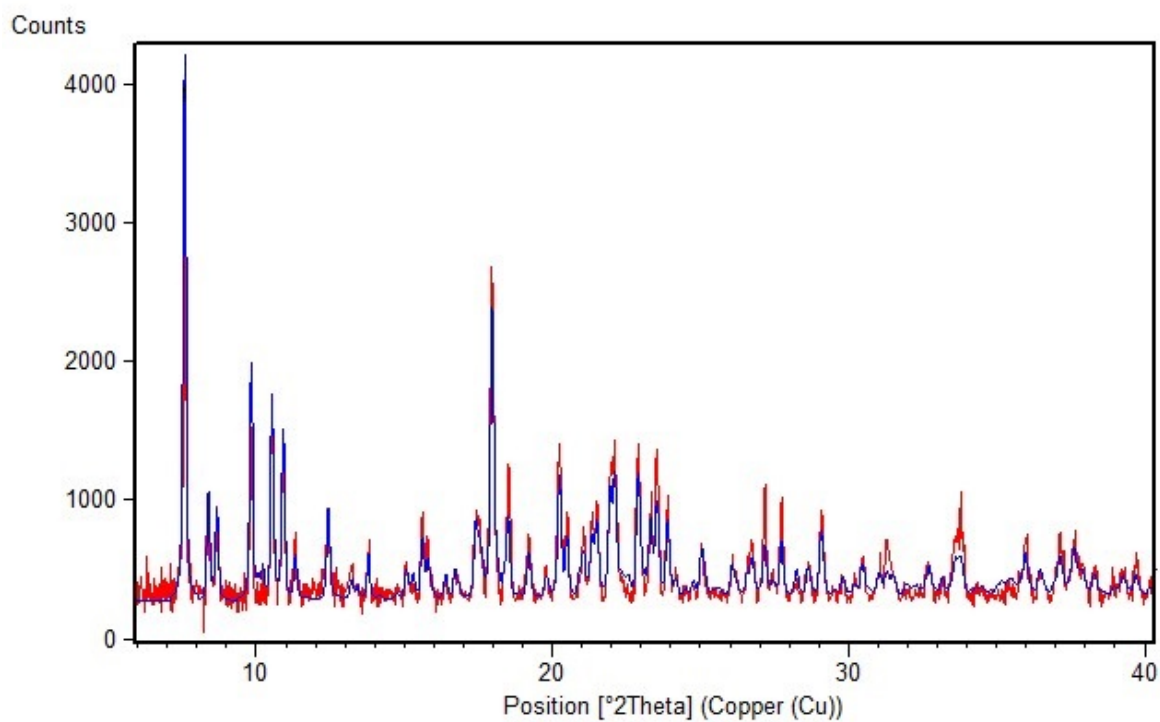


Figure S2: X-ray powder pattern of **2**. (red: observed, blue: simulated).

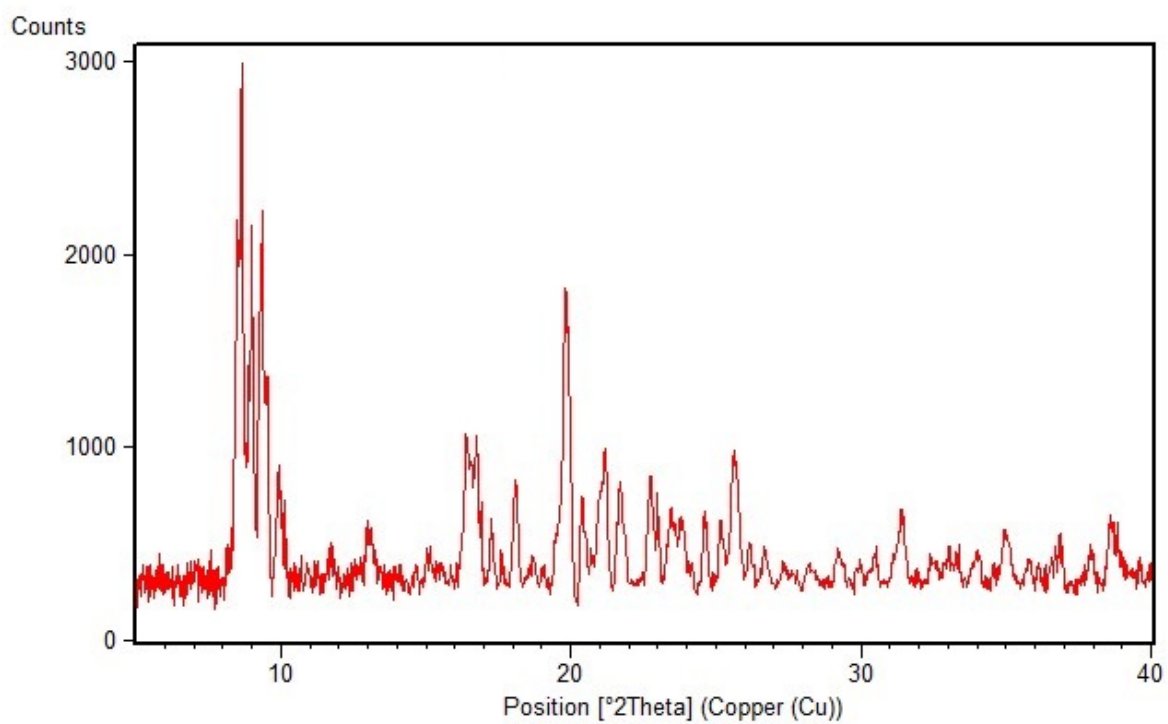


Figure S3: X-ray powder pattern of **3**.

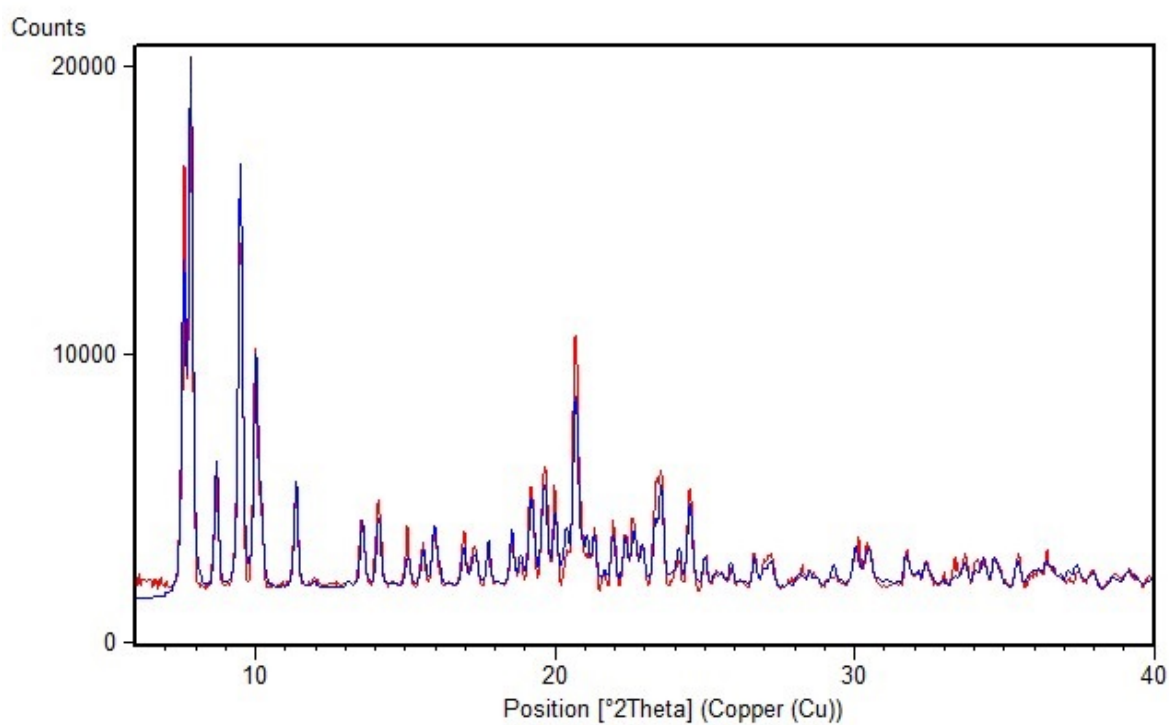


Figure S4: X-ray powder pattern of **4**. (red: observed, blue: simulated).

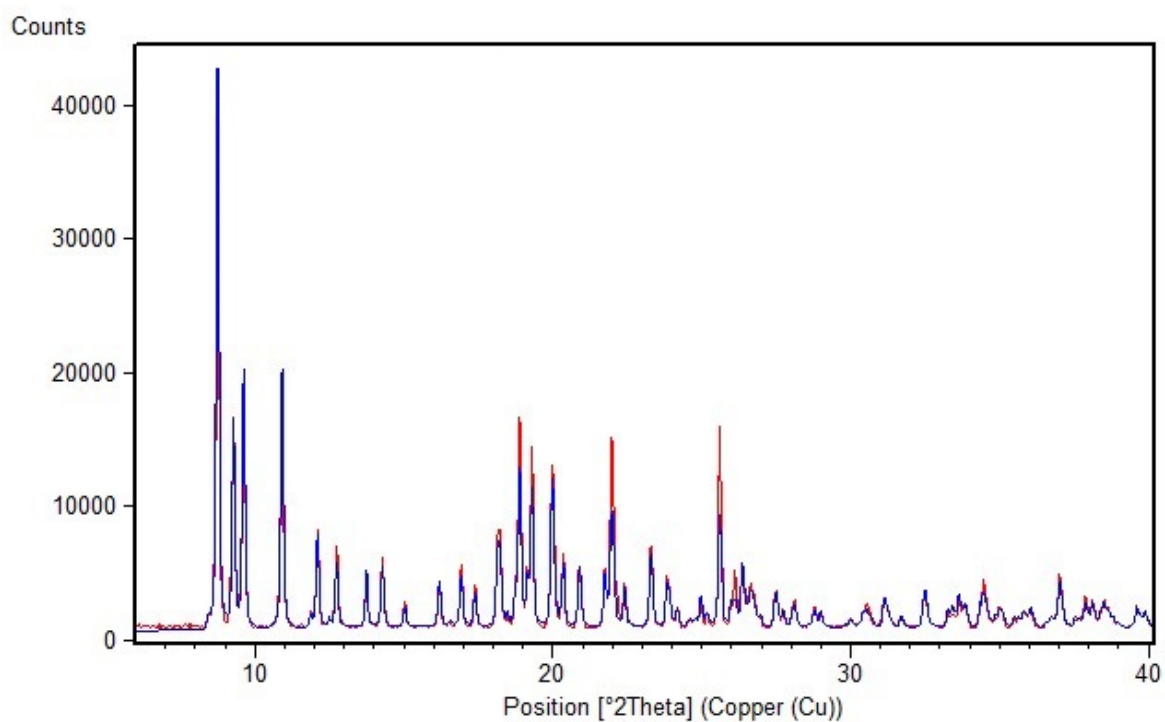


Figure S5: X-ray powder pattern of **5**. (red: observed, blue: simulated).

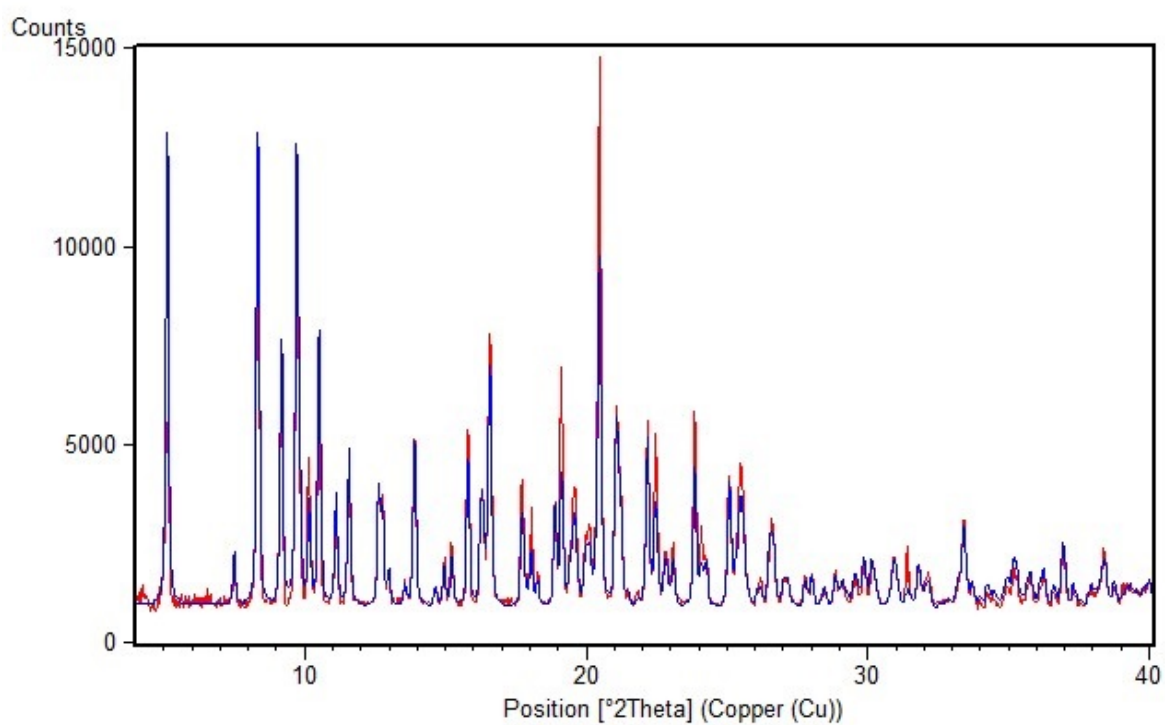


Figure S6: X-ray powder pattern of **6**. (red: observed, blue: simulated).

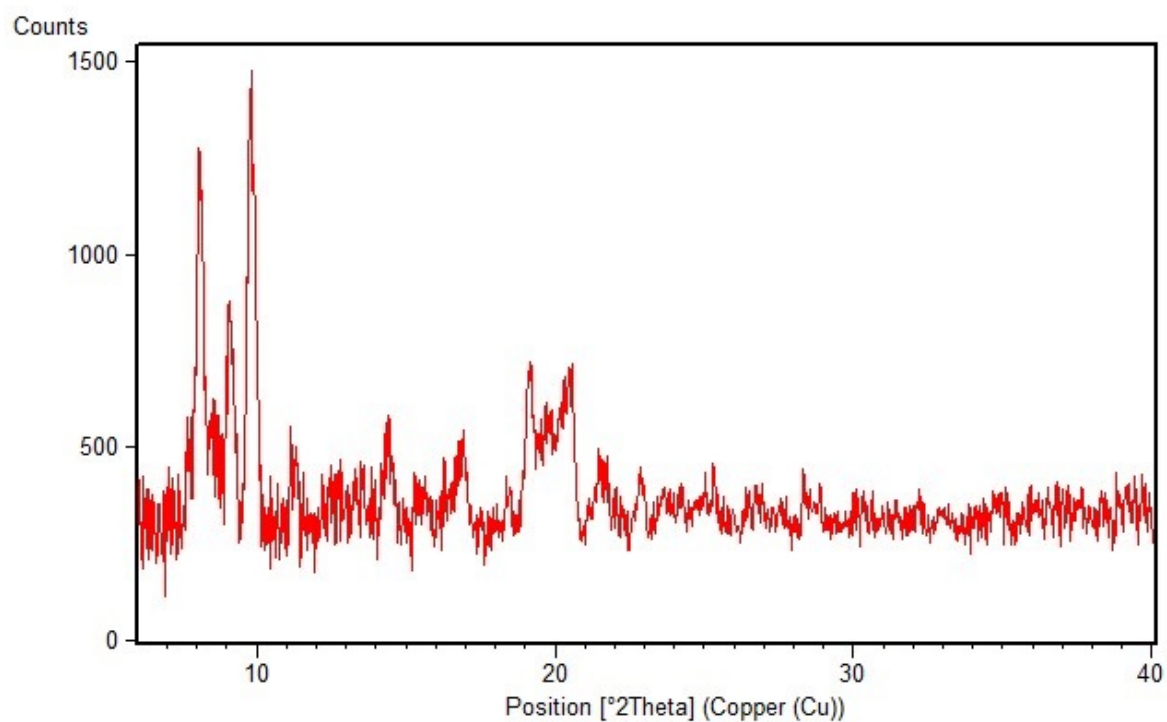


Figure S7: X-ray powder pattern of **7**.

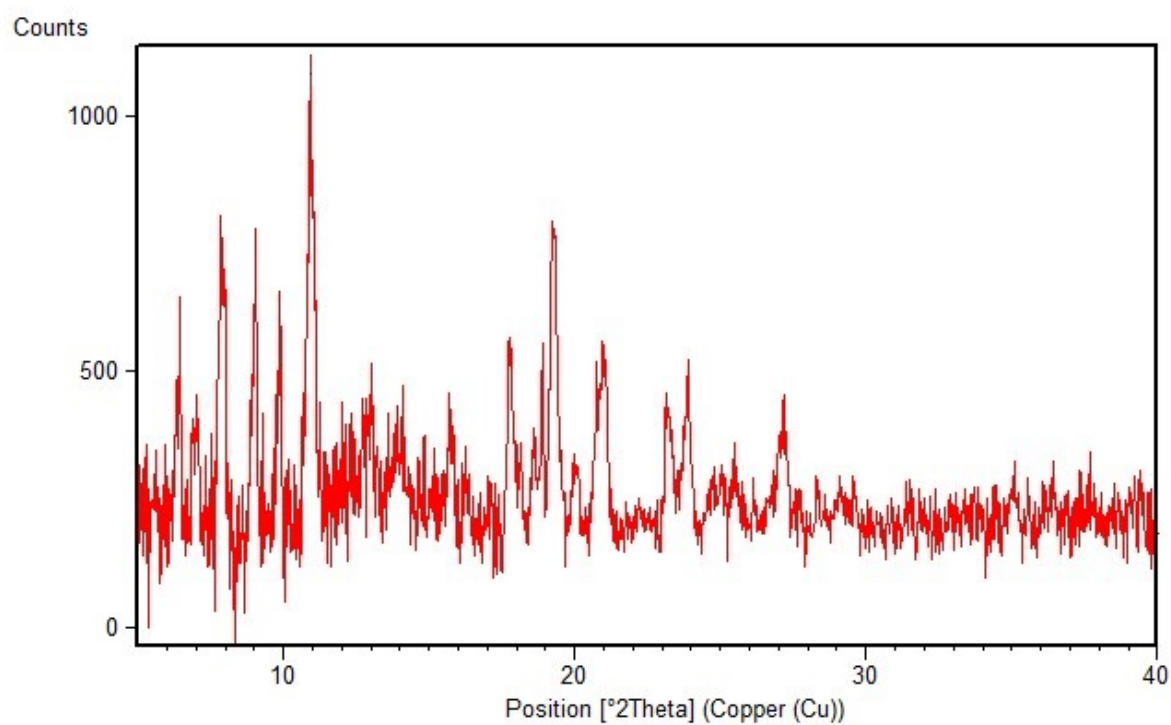


Figure S8: X-ray powder pattern of **8**.

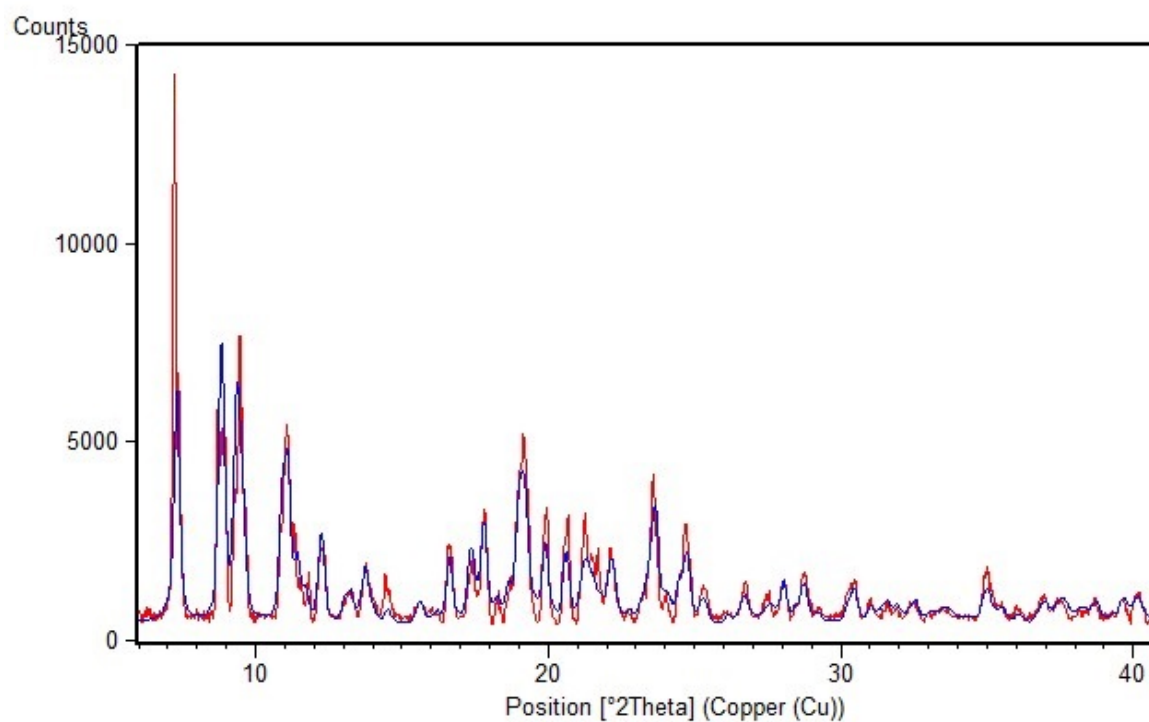


Figure S9: X-ray powder pattern of **9**. (red: observed, blue: simulated).

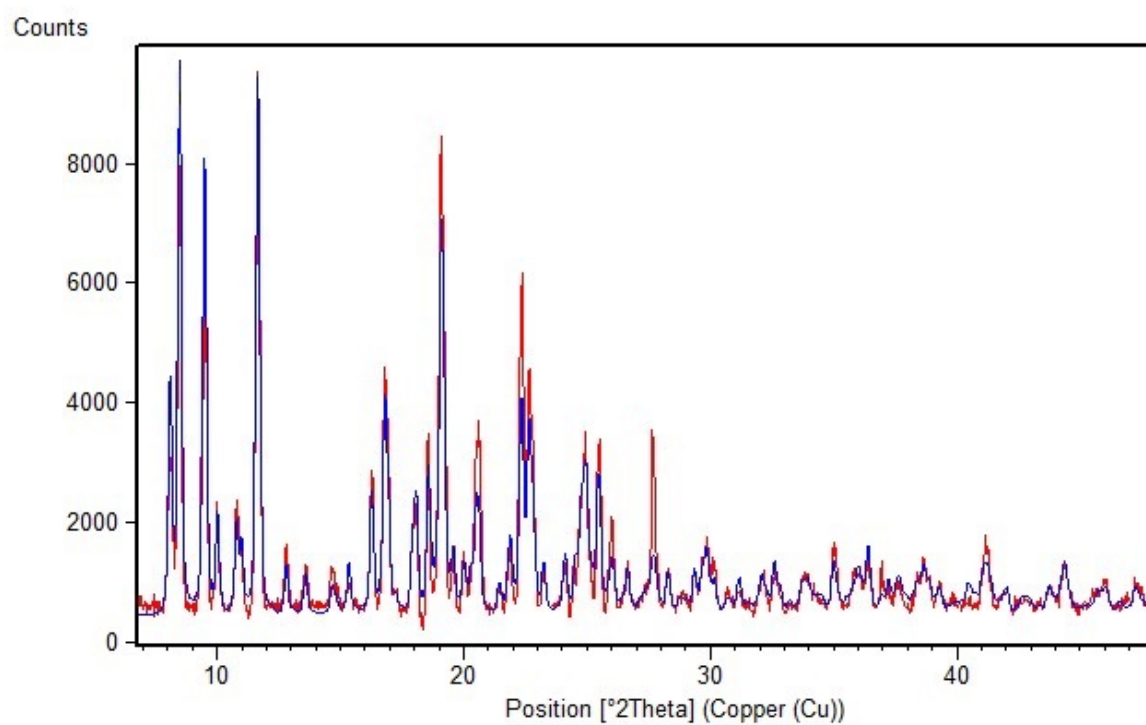


Figure S10: X-ray powder pattern of **10**. (red: observed, blue: simulated).

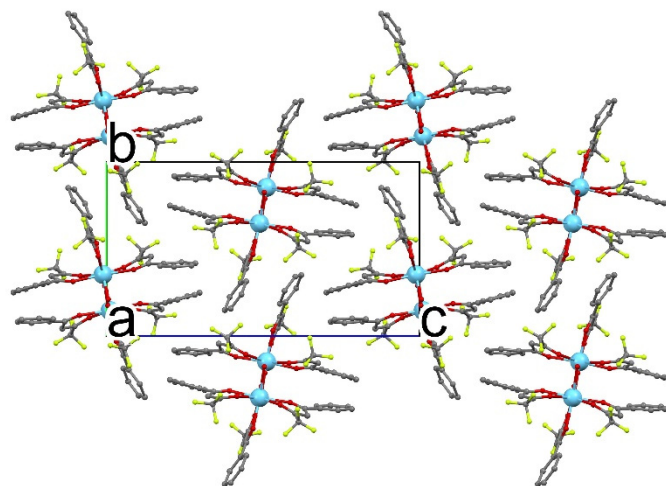


Figure S11: Packing plot of 1.

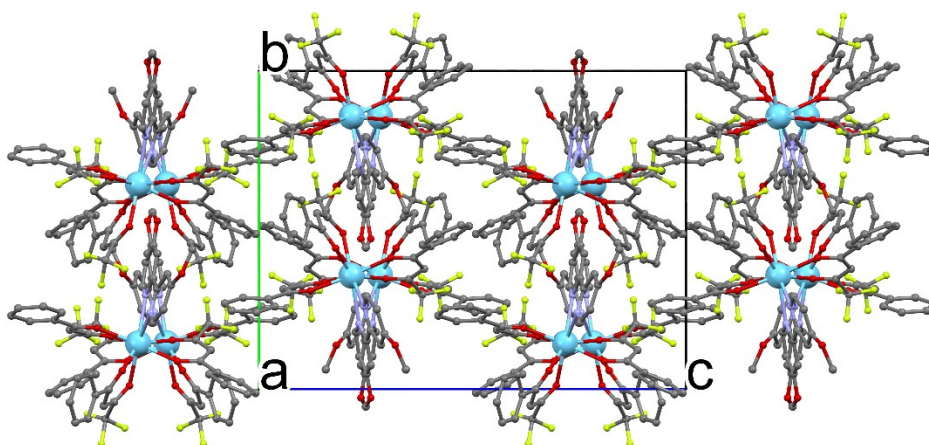


Figure S12: Packing plot of 2.

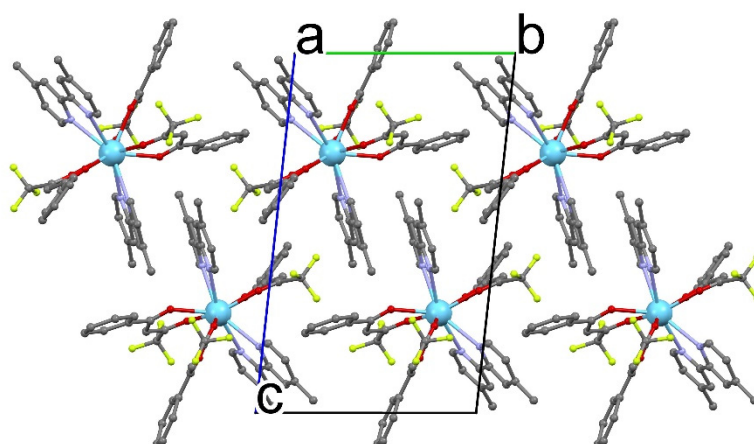


Figure S13: Packing plot of 3.

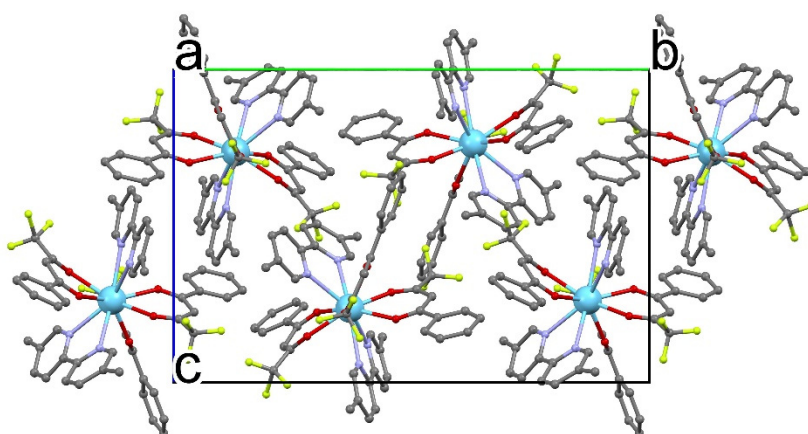


Figure S14: Packing plot of **4**.

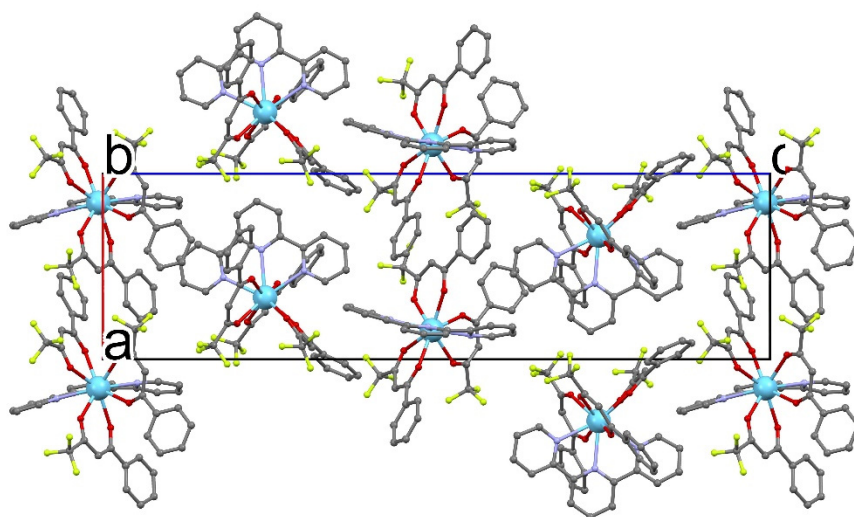


Figure S15: Packing plot of **5**.

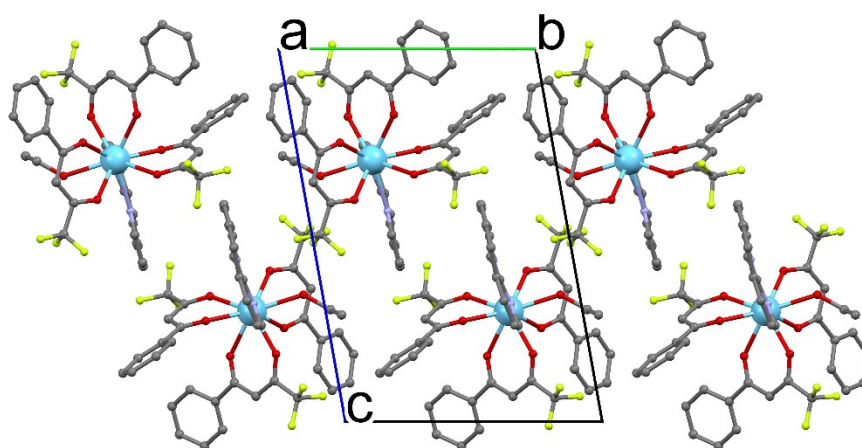


Figure S16: Packing plot of **6**.

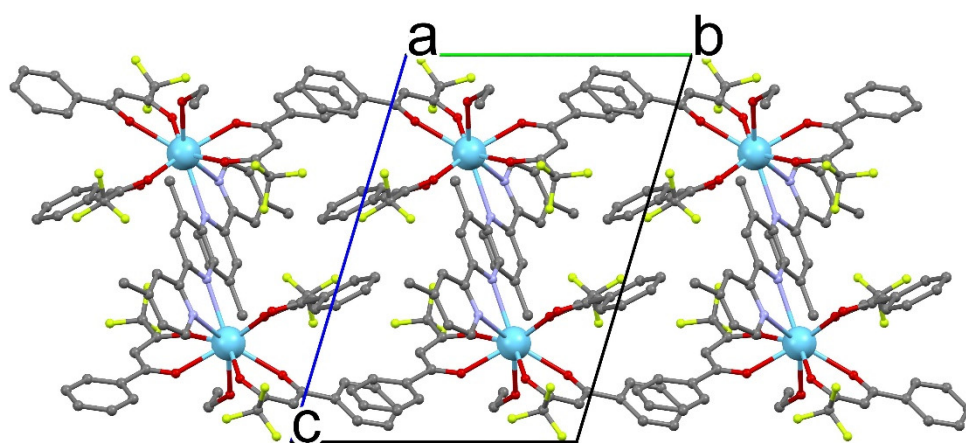


Figure S17: Packing plot of **7**.

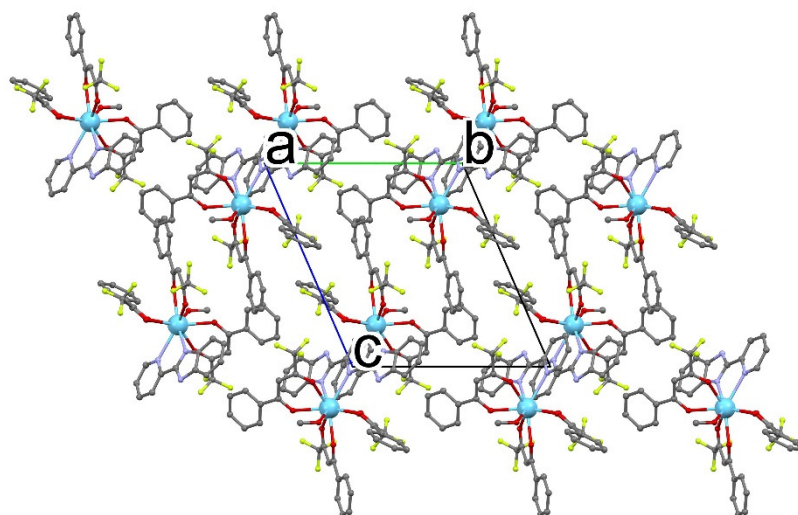


Figure S18: Packing plot of **8**.

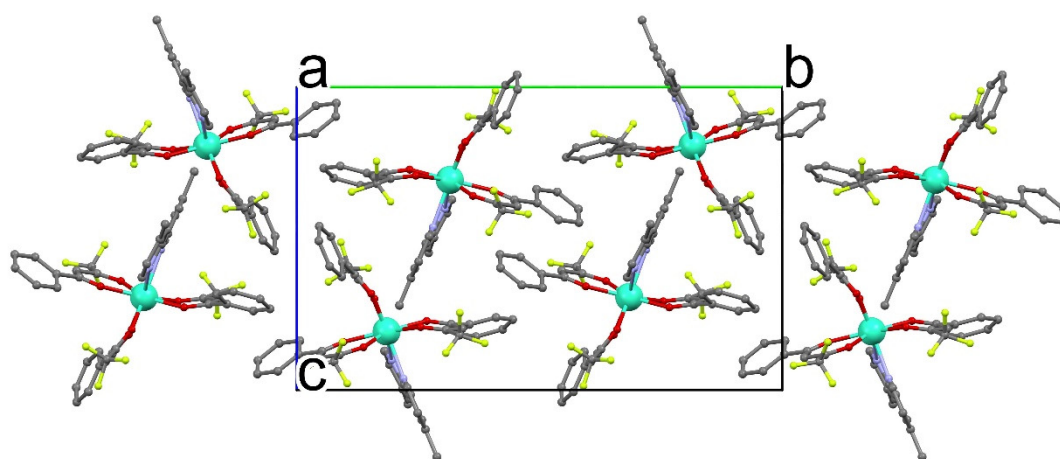


Figure S19: Packing plot of **9**.

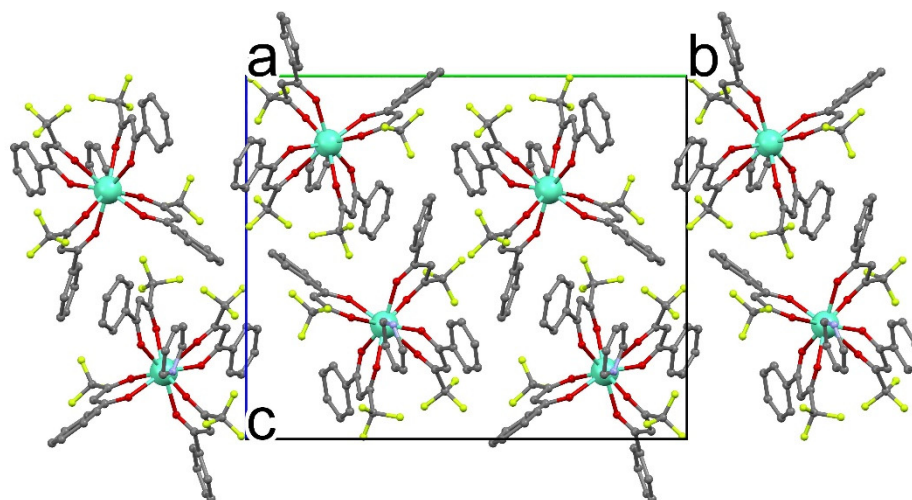


Figure S20: Packing plot of **10**.

Table S1: Selected bond distances (Å) and bond angles (°) of **1 – 10**.

Compound 1:

La1-O1 2.486(3), La1-O2 2.445(3), La1-O3 2.488(2), La1-O4 2.444(3), La1-O5 2.540(2), La1-O6 2.407(3), La1-O7 2.564(3), La1-O8 2.517(2); O1-La1-O2 68.64(9), O3-La1-O4 68.68(9), O5-La1-O6 68.43(8), O7-La1-O8 66.08(9).

Compound 2:

La1-O1 2.4642(12), La1-O2 2.4549(12), La1-O3 2.4688(13), La1-O4 2.4824(12), La1-O5 2.4623(12), La1-O6 2.4859(12), La1-N1 2.6687(15), La1-N2 2.6690(14); O1-La1-O2 69.08(4), O3-La1-O4 69.26(4), O5-La1-O6 68.68(4), N1-La1-N2 59.86(4).

Compound 3:

La1-O1 2.5073(14), La1-O2 2.5045(15), La1-O3 2.4911(14), La1-O4 2.5298(14), La1-O5 2.5115(14), La1-O6 2.5732(15), La1-N1 2.8299(17), La1-N2 2.8091(16), La1-N3 2.8434(18), La1-N4 2.8637(18); O1-La1-O2 67.64(5), O3-La1-O4 67.95(5), O5-La1-O6 67.46(5), N1-La1-N2 57.08(5), N3-La1-N4 55.86(5).

Compound 4:

La1-O1 2.5121(15), La1-O2 2.5115(16), La1-O3 2.5254(16), La1-O4 2.5733(15), La1-O5 2.5173(15), La1-O6 2.5659(15), La1-N1 2.751(2), La1-N2 2.8216(18), La1-N3 2.8010(19), La1-N4 2.804(2); O1-La1-O2 68.32(5), O3-La1-O4 65.96(5), O5-La1-O6 66.07(5), N1-La1-N2 58.38(6), N3-La1-N4 57.03(6).

Compound 5:

La1-O1 2.480(2), La1-O2 2.481(3), La1-O3 2.555(3), La1-O4 2.514(2), La1-O5 2.453 (3), La1-O6 2.495(2), La1-N1 2.709(3), La1-N2 2.744(3), La1-N3 2.705(3); O1-La1-O2 69.66(8), O3-La1-O4 71.56(9), O5-La1-O6 69.40(8), N1-La1-N2 61.01(9), N2-La1-N3 59.83(9).

Compound 6:

La1-O1 2.4588(17), La1-O2 2.5221(16), La1-O3 2.5090(16), La1-O4 2.4788(17), La1-O5 2.5107(18), La1-O6 2.5143(15), La1-O7 2.6229(17), La1-N1 2.7736(18), La1-N2 2.742(2); O1-La1-O2 69.05(5), O3-La1-O4 68.55(5), O5-La1-O6 66.93(5), N1-La1-N2 59.74(6).

Compound 7:

La1-O1 2.4891(16), La1-O2 2.5030(16), La1-O3 2.4799(16), La1-O4 2.4889(17), La1-O5 2.4790(10), La1-O6 2.5658(18), La1-O7 2.623(2), La1-N1 2.755(2), La1-N2 2.735(2); O1-La1-O2 67.74(5), O3-La1-O4 70.60(6), O5-La1-O6 67.49(6), N1-La1-N2 58.53(6).

Compound 8:

La1-O1 2.485(2), La1-O2 2.533(2), La1-O3 2.581(2), La1-O4 2.478(2), La1-O5 2.498(2), La1-O6 2.481(2), La1-O7 2.668(2), La1-N1 2.745(3), La1-N2 2.658(3); O1-La1-O2 67.35(7), O3-La1-O4 67.18(6), O5-La1-O6 67.85(7), N1-La1-N2 61.40(7).

Compound 9:

Tb1-O1 2.354(3), Tb1-O2 2.340(3), Tb1-O3 2.370(3), Tb1-O4 2.317(3), Tb1-O5 2.366(3), Tb1-O6 2.317(3), Tb1-N1 2.547(3), Tb1-N2 2.530(3); O1-Tb1-O2 71.47(10), O3-Tb1-O4 71.33(10), O5-Tb1-O6 72.12(10), N1-Tb1-N2 63.08(10).

Compound 10:

Eu1-O1 2.381(6), Eu1-O2 2.403(5), Eu1-O3 2.451(5), Eu1-O4 2.346(6), Eu1-O5 2.362(6), Eu1-O6 2.364(5), Eu1-O7 2.388(6), Eu1-O8 2.361(6); O1-Eu1-O2 72.14(19), O3-Eu1-O4 70.81(18), O5-Eu1-O6 73.0(2), O7-Eu1-O8 72.1(2).

Table S2: Non-coordinative interactions in **1**.

6-Membered Ring (1) C5 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (2) C15 --> C16 --> C17 --> C18 --> C19 --> C20 -->
 6-Membered Ring (3) C25 --> C26 --> C27 --> C28 --> C29 --> C30 -->

Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.0 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp
Cg1	Cg2	[2665]	4.737(3)	19.8(3)	39.4	30.2	4.0945(19)	3.663(2)
Cg1	Cg2	[3466]	5.705(3)	14.7(3)	57.5	63.0	2.5897(19)	3.069(2)
Cg1	Cg3	[3556]	5.434(3)	62.1(2)	35.8	82.2	0.7342(19)	4.4085(18)
Cg2	Cg1	[2664]	4.737(3)	19.8(3)	30.2	39.4	3.663(2)	4.0945(19)
Cg3	Cg1	[2664]	5.294(3)	54.3(2)	35.9	65.1	2.2308(18)	4.2907(19)
Cg3	Cg2	[4645]	5.419(3)	42.4(3)	42.6	79.3	1.0060(18)	3.990(2)

[2665]	3/2-X,1-Y,1/2+Z
[3466]	-1/2+X,3/2-Y,1-Z
[3556]	1/2+X,1/2-Y,1-Z
[2664]	3/2-X,1-Y,-1/2+Z
[4645]	1-X,-1/2+Y,1/2-Z

Analysis of X-H...Cg(Pi-Ring) Interactions (H...Cg < 4.0 Ang. - Gamma < 30.0 Deg)

Y--X(I)	Cg(J)	[ARU(J)]	X..Cg	X-Perp	Gamma	Y-X..Cg	Y..Cg	Y-X,Pi
C11-F6	Cg1	[3466]	3.769(4)	3.743	6.82	99.8(2)	4.203(4)	3.62
C21-F8	Cg3	[3556]	3.428(4)	3.351	12.18	105.0(2)	3.979(5)	25.69
C21-F9	Cg3	[3556]	3.859(4)	3.598	21.20	85.3(3)	3.979(5)	14.09

[3466]	-1/2+X,3/2-Y,1-Z
[3556]	1/2+X,1/2-Y,1-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0.8488(2)	0.58920(15)	0.72723(8)
Cg2	0.87570(18)	0.71947(18)	0.25780(8)
Cg3	0.46492(18)	0.273227(14)	0.41246(9)

Table S3: Non-coordinative interactions in 2.

6-Membered Ring (1) N1 --> C31 --> C32 --> C33 --> C34 --> C35 -->
 6-Membered Ring (2) N2 --> C36 --> C37 --> C38 --> C39 --> C40 -->
 6-Membered Ring (3) C5 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (4) C15 --> C16 --> C17 --> C18 --> C19 --> C20 -->
 6-Membered Ring (5) C25 --> C26 --> C27 --> C28 --> C29 --> C30 -->

Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.0 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	Cg4	[7655]	3,9547(11)	3,3055	16,40(9)	19,1	34	3,2774(7)	3,7379(8)
Cg1	Cg5	[7655]	5,3385(11)	21,6968	75,39(9)	50,5	45,5	3,7407(7)	3,3968(8)
Cg2	Cg3	[8565]	4,9097(10)	-16,8341	67,05(9)	15	82	0,6841(7)	4,7435(8)
Cg2	Cg5	[1555]	5,9840(11)	19,7705	86,97(9)	32,6	64,9	2,5341(7)	5,0405(8)
Cg3	Cg4	[1555]	5,6589(12)	19,3295	75,23(10)	28,5	47	3,8577(8)	4,9711(9)
Cg3	Cg4	[7655]	5,6048(12)	3,3055	88,15(10)	31,6	56,7	3,0804(8)	4,7718(9)
Cg3	Cg5	[2664]	4,6103(12)	-5,8977	37,92(10)	35,5	36,4	3,7106(9)	3,7522(8)
Cg3	Cg5	[8564]	4,3550(12)	-7,824	26,00(10)	28,1	21,6	4,0481(9)	3,8404(8)
Cg4	Cg1	[7645]	3,9547(11)	18,8969	16,40(9)	34	19,1	3,7379(8)	3,2774(7)
Cg4	Cg3	[1555]	5,6589(12)	7,4051	75,23(10)	47	28,5	4,9710(9)	3,8576(8)
Cg4	Cg3	[7645]	5,6050(12)	8,5858	88,15(10)	56,7	31,6	4,7719(9)	3,0804(8)
Cg4	Cg5	[2664]	4,9613(12)	-5,8977	67,13(10)	18,1	79	0,9465(9)	4,7160(8)
Cg5	Cg1	[7645]	5,3387(11)	18,8969	75,39(9)	45,5	50,5	3,3968(8)	3,7408(7)
Cg5	Cg2	[7645]	5,9995(11)	18,4006	81,32(9)	21,7	61	2,9044(8)	5,5734(7)
Cg5	Cg3	[2665]	4,6103(12)	0,6406	37,92(10)	36,4	35,5	3,7522(8)	3,7106(9)
Cg5	Cg3	[8565]	4,3550(12)	-16,8341	26,00(10)	21,6	28,1	3,8404(8)	4,0481(9)

[7655]	3/2-X,1/2+Y,Z	[8564]	X,3/2-Y,-1/2+Z
[8565]	X,3/2-Y,1/2+Z	[7645]	3/2-X,-1/2+Y,Z
[1555]	X,Y,Z	[2665]	3/2-X,1-Y,1/2+Z
[2664]	3/2-X,1-Y,-1/2+Z		

Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 40.0 Deg)

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- X-H..Cg = X-H-Cg angle (degrees)
- X..Cg = Distance of X to Cg (Angstrom)
- X-H, Pi = Angle of the X-H bond with the Pi-plane (i.e. ' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C9-H9	Cg2	[8564]	2,98	2,79	20,25	135	3,708(2)	57

[8564]	X,3/2-Y,-1/2+Z
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Analysis of Y-X...Cg(Pi-Ring) Interactions (X...Cg < 4.0 Ang. - Gamma < 30.0 Deg)

Y--X(I)	Cg(J)	[ARU(J)]	X..Cg	X-Perp	Gamma	Y-X..Cg	Y..Cg	Y-X,Pi
C21-F8	Cg1	[1555]	3,7704(15)	3,574	18,55	124,48(11)	4,661(2)	19,05
C11-F5	Cg2	[7645]	3,530(19)	-3,49	9,02	102,9(9)	4,122(2)	14,7

[1555]	X,Y,Z
[7645]	3/2-X,-1/2+Y,Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,62736(3)	0,87298(4)	0,74353(3)
Cg2	0,81388(3)	0,78356(4)	0,76879(3)
Cg3	0,76795(4)	0,73570(5)	0,47842(3)
Cg4	0,87832(4)	0,47005(5)	0,58699(4)
Cg5	0,79458(4)	0,51743(5)	0,93762(3)

Table S4: Non-coordinative interactions in **3**.

6-Membered Ring (1) N1 --> C31 --> C32 --> C33 --> C34 --> C35 -->
 6-Membered Ring (2) N2 --> C36 --> C37 --> C38 --> C39 --> C40 -->
 6-Membered Ring (3) N3 --> C43 --> C44 --> C45 --> C46 --> C47 -->
 6-Membered Ring (4) N4 --> C48 --> C49 --> C50 --> C51 --> C52 -->
 6-Membered Ring (5) C5 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (6) C15 --> C16 --> C17 --> C18 --> C19 --> C20 -->
 6-Membered Ring (7) C25 --> C26 --> C27 --> C28 --> C29 --> C30 -->

Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.0 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	Cg1	[2566]	4,8577(12)	0,5845	0,04(10)	48,8	48,8	3,2028(8)	3,2028(8)
Cg1	Cg2	[2566]	4,4470(12)	-0,1677	6,15(10)	39,2	41,3	3,3393(8)	3,4477(8)
Cg1	Cg5	[2676]	4,6783(12)	-12,7065	54,65(10)	16,6	70,3	1,5772(8)	4,4833(9)
Cg2	Cg1	[2566]	4,4470(12)	0,5845	6,15(10)	41,3	39,2	3,4477(8)	3,3393(8)
Cg2	Cg5	[1555]	5,2527(13)	14,9964	52,63(10)	44,8	37,4	4,1737(8)	3,7291(9)
Cg2	Cg5	[2676]	5,6484(13)	-12,7065	52,63(10)	36,3	70,5	1,8837(8)	4,5529(9)
Cg3	Cg3	[2677]	5,5589(13)	7,5211	0,03(10)	51,6	51,6	3,4507(9)	3,4506(9)
Cg3	Cg4	[2677]	4,9151(13)	5,1305	7,20(11)	43,8	51	3,0961(9)	3,5491(9)
Cg3	Cg5	[1555]	5,8645(13)	14,9964	79,12(10)	34,2	68,7	2,1307(9)	4,8478(9)
Cg3	Cg6	[1555]	5,7604(14)	11,0817	63,31(11)	16,8	53,9	3,3915(9)	5,5141(9)
Cg3	Cg7	[1665]	5,0074(13)	16,6017	62,29(11)	13,6	74,7	1,3195(9)	4,8675(10)
Cg4	Cg3	[2677]	4,9151(13)	7,5211	7,20(11)	51	43,8	3,5491(9)	3,0960(9)
Cg5	Cg1	[1655]	5,6671(14)	4,6286	54,65(10)	57,2	67,6	2,1550(9)	3,0731(8)
Cg5	Cg2	[1555]	5,2528(13)	3,3151	52,63(10)	37,4	44,8	3,7291(9)	4,1737(8)
Cg5	Cg7	[1665]	4,2536(13)	16,6017	38,74(11)	14,2	28,5	3,7365(9)	4,1243(9)
Cg6	Cg3	[1555]	5,7603(14)	-4,0705	63,31(11)	53,9	16,8	5,5141(9)	3,3915(9)
Cg6	Cg3	[2677]	5,1557(13)	7,5211	63,31(11)	14	66,4	2,0635(9)	5,0022(9)
Cg6	Cg4	[2677]	5,3453(15)	5,1305	57,30(11)	33,2	61,2	2,5711(9)	4,4718(9)
Cg6	Cg6	[2567]	5,0238(16)	-8,0029	0,00(11)	52,2	52,2	3,0789(9)	3,0789(9)
Cg7	Cg1	[2566]	5,8194(13)	0,5845	87,10(11)	25,4	62,7	2,6703(9)	5,2554(8)
Cg7	Cg2	[2566]	5,8523(13)	-0,1677	89,97(11)	43,8	64,4	2,5269(9)	4,2266(8)
Cg7	Cg5	[1445]	4,2537(13)	5,4565	38,74(11)	28,5	14,2	4,1243(9)	3,7366(9)
Cg7	Cg6	[2567]	4,7463(14)	-8,0029	54,57(11)	19,6	67,3	1,8318(9)	4,4719(9)

[2566]	-X,1-Y,1-Z
[2676]	1-X,2-Y,1-Z
[1555]	X,Y,Z
[2677]	1-X,2-Y,2-Z
[1665]	1+X,1+Y,Z

[1655]	1+X,Y,Z
[2567]	-X,1-Y,2-Z
[1445]	-1+X,-1+Y,Z

Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 40.0 Deg)

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- X-H..Cg = X-H-Cg angle (degrees)
- X..Cg = Distance of X to Cg (Angstrom)
- X-H, Pi = Angle of the X-H bond with the Pi-plane (i.e. ' Perpendicular = 90 degrees, Parallel = 0 degrees)

X-H(I)	Cg(J)	[ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C9-H9	Cg1	[2676]	2,63	2,6	7,9	141	3,413(2)	53
C19-H19	Cg7	[2567]	2,75	2,69	10,98	138	3,510(3)	50
C41-H41C	Cg2	[2566]	2,9	-2,74	18,91	117	3,458(2)	46

[2676]	1-X,2-Y,1-Z
[2567]	-X,1-Y,2-Z
[2566]	-X,1-Y,1-Z

Analysis of Y-X...Cg(Pi-Ring) Interactions (X..Cg < 4.0 Ang. - Gamma < 30.0 Deg)

Y-X(I)	Cg(J)	[ARU(J)]	X..Cg	X-Perp	Gamma	Y-X..Cg	Y..Cg	Y-X,Pi
C1-F1	Cg4	[1555]	3,9453(19)	3,515	27	112,00(12)	4,614(3)	0,04
C1-F3	Cg5	[2676]	3,6259(17)	-3,405	20,09	108,96	4,256(3)	0,25

[1555]	X,Y,Z
[2676]	1-X,2-Y,1-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,00623(8)	0,69205(7)	0,53857(4)
Cg2	0,33731(8)	0,63982(7)	0,52661(4)
Cg3	0,60109(8)	0,95710(8)	0,87916(5)
Cg4	0,30838(9)	1,07223(8)	0,86330(5)
Cg5	0,77363(8)	1,00351(8)	0,59525(5)
Cg6	0,23647(10)	0,60517(8)	1,02184(5)
Cg7	-0,12680(10)	0,29409(8)	0,75494(5)

Table S5: Non-coordinative interactions in **4**.

6-Membered Ring (1) N1 --> C31 --> C32 --> C33 --> C34 --> C35 -->
 6-Membered Ring (2) N2 --> C37 --> C38 --> C39 --> C40 --> C41 -->
 6-Membered Ring (3) N3 --> C43 --> C44 --> C45 --> C46 --> C47 -->
 6-Membered Ring (4) N4 --> C49 --> C50 --> C51 --> C52 --> C53 -->
 6-Membered Ring (5) C5 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (6) C15 --> C16 --> C17 --> C18 --> C19 --> C20 -->
 6-Membered Ring (7) C25 --> C26 --> C27 --> C28 --> C29 --> C30 -->

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.0 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	Cg5	[1555]	5,7119(14)	12,1492	48,71(12)	13,8	47,5	3,8624(10)	5,5472(10)
Cg1	Cg7	[2655]	4,2310(14)	-2,8647	41,92(12)	7,7	49,2	2,7649(11)	4,1927(10)
Cg2	Cg6	[1555]	5,1314(15)	12,2081	62,56(12)	9,8	58,9	2,6471(10)	5,0563(10)
Cg2	Cg6	[4565]	5,1783(15)	3,3691	9,74(12)	45,8	45,6	3,6214(10)	3,6079(10)
Cg3	Cg1	[4464]	4,9280(14)	-14,6495	58,92(12)	15,7	74,1	1,3519(10)	4,7438(10)
Cg3	Cg3	[3665]	5,1034(14)	-7,6555	0,00(12)	50,9	50,9	3,2209(10)	3,2210(10)
Cg3	Cg4	[3665]	4,0648(14)	-6,9121	5,21(11)	33,1	35,7	3,3020(10)	3,4053(10)
Cg3	Cg6	[1555]	5,6209(14)	12,2081	80,78(12)	40,1	51,4	3,5088(10)	4,3011(10)
Cg4	Cg3	[3665]	4,0649(14)	-7,6555	5,21(11)	35,7	33,1	3,4052(10)	3,3020(10)
Cg4	Cg6	[4564]	5,4299(15)	-8,6992	42,53(12)	57,4	41	4,0995(10)	2,9226(10)
Cg4	Cg7	[1555]	5,9906(15)	9,767	81,82(12)	21,5	60,3	2,9677(10)	5,5721(10)
Cg5	Cg1	[1555]	5,7119(14)	6,5906	48,71(12)	47,5	13,8	5,5472(10)	3,8624(10)
Cg5	Cg5	[3766]	4,8865(15)	-8,7339	0,03(11)	45,7	45,7	3,4152(10)	3,4153(10)
Cg5	Cg6	[4565]	4,9669(14)	3,3691	78,47(12)	10,5	80,5	0,8166(10)	4,8835(10)
Cg6	Cg1	[4464]	4,6669(15)	-14,6495	31,58(12)	29,7	60,4	2,3047(10)	4,0527(11)
Cg6	Cg2	[1555]	5,1313(15)	-1,0201	62,56(12)	58,9	9,8	5,0563(10)	2,6470(10)
Cg6	Cg2	[4464]	5,1784(15)	9,8164	9,74(12)	45,6	45,8	3,6080(10)	3,6215(10)
Cg6	Cg3	[1555]	5,6210(14)	10,8764	80,78(12)	51,4	40,1	4,3011(10)	3,5088(10)
Cg6	Cg4	[4465]	5,4299(15)	-21,2497	42,53(12)	41	57,4	2,9226(10)	4,0995(10)
Cg6	Cg7	[2655]	5,9745(15)	-2,8647	42,95(12)	46,2	62,4	2,7643(11)	4,1350(11)
Cg7	Cg1	[2645]	4,2311(14)	9,9263	41,92(12)	49,2	7,7	4,1928(10)	2,7650(11)
Cg7	Cg3	[3665]	5,0469(15)	-7,6555	82,87(12)	22	65,5	2,0960(10)	4,6781(10)
Cg7	Cg5	[3766]	4,8041(15)	-8,7339	64,67(12)	13	70,7	1,5861(10)	4,6804(10)

[1555]	X,Y,Z
[2655]	3/2-X,1/2+Y,1/2-Z
[4565]	1/2+X,3/2-Y,1/2+Z
[4464]	-1/2+X,3/2-Y,-1/2+Z
[3665]	1-X,1-Y,-Z

[4564]	1/2+X,3/2-Y,-1/2+Z
[3766]	2-X,1-Y,1-Z
[4465]	-1/2+X,3/2-Y,1/2+Z
[2645]	3/2-X,-1/2+Y,1/2-Z

Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 40.0 Deg)

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- X-H..Cg = X-H-Cg angle (degrees)
- X..Cg = Distance of X to Cg (Angstrom)
- X-H, Pi = Angle of the X-H bond with the Pi-plane (i.e. ' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C7-H7	Cg7	[3766]	2,83	2,8	8,49	137	3,585(3)	54
C16-H16	Cg5	[4464]	2,9	2,88	6,52	143	3,708(3)	59
C29-H29	Cg1	[2645]	2,98	2,72	24,49	105	3,351(3)	39
C32-H32	Cg6	[4565]	2,92	-2,9	5,89	125	3,552(3)	29
C33-H33	Cg3	[4565]	2,77	2,77	2,03	149	3,618(3)	57

[3766]	2-X,1-Y,1-Z
[4464]	-1/2+X,3/2-Y,-1/2+Z
[2645]	3/2-X,-1/2+Y,1/2-Z
[4565]	1/2+X,3/2-Y,1/2+Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,75904(7)	0,75604(4)	0,40758(7)
Cg2	0,50485(7)	0,67682(4)	0,44873(7)
Cg3	0,39767(7)	0,57206(4)	0,06871(7)
Cg4	0,65311(7)	0,59984(4)	-0,02858(7)
Cg5	0,87894(7)	0,54238(4)	0,57635(7)
Cg6	0,27209(7)	0,77775(4)	0,20810(7)
Cg7	0,87226(7)	0,41339(5)	0,18479(7)

Table S6: Non-coordinative interactions in **5**.

6-Membered Ring (1) N1 --> C31 --> C32 --> C33 --> C34 --> C35 -->
 6-Membered Ring (2) N2 --> C36 --> C37 --> C38 --> C39 --> C40 -->
 6-Membered Ring (3) N3 --> C41 --> C42 --> C43 --> C44 --> C45 -->
 6-Membered Ring (4) C5 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (5) C15 --> C16 --> C17 --> C18 --> C19 --> C20 -->
 6-Membered Ring (6) C25 --> C26 --> C27 --> C28 --> C29 --> C30 -->

Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.000 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- Cgl_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	Cgl_Perp	CgJ_Perp	Slippage
Cg1	Cg3	[2655]	5,544(2)	0,0627	73,1(2)	39,6	63,5	2,4771(18)	4,2723(17)
Cg1	Cg6	[1555]	5,494(2)	19,953	85,8(2)	11,5	74,4	1,4736(17)	5,3834(17)
Cg1	Cg6	[1655]	5,331(2)	21,8139	85,8(2)	22,8	85,8	0,3872(17)	4,9156(17)
Cg2	Cg4	[1455]	5,649(3)	17,4352	68,1(2)	28,9	63,4	2,5291(17)	4,9451(16)
Cg2	Cg4	[1555]	5,528(3)	21,6492	68,1(2)	8,3	72,3	1,6849(17)	5,4700(16)
Cg2	Cg5	[1545]	5,639(2)	-7,9962	64,5(2)	55,2	32,3	4,7640(16)	3,2150(15)
Cg3	Cg4	[1455]	5,028(2)	17,4352	80,8(2)	12,5	85	0,4348(16)	4,9078(16)
Cg3	Cg5	[4564]	3,762(2)	2,5945	20,53(18)	27,9	7,4	3,7303(16)	3,3250(15)
Cg4	Cg1	[4664]	5,538(2)	-4,2934	64,4(2)	37	67,9	2,0823(17)	4,4204(17)
Cg4	Cg5	[4564]	5,115(2)	2,5945	83,03(19)	24,4	79,4	0,9366(17)	4,6564(15)
Cg4	Cg6	[1655]	3,968(3)	21,8139	18,7(2)	25,7	27,8	3,5112(18)	3,5756(18)
Cg5	Cg1	[1565]	5,155(2)	6,5867	88,5(2)	22,3	74,7	1,3645(15)	4,7708(18)
Cg5	Cg2	[1565]	5,639(2)	9,0919	64,5(2)	32,3	55,2	3,2150(15)	4,7640(16)
Cg5	Cg2	[2655]	5,641(2)	4,8282	31,8(2)	48,6	61,5	2,6944(15)	3,7290(19)
Cg5	Cg3	[2655]	3,762(2)	0,0627	20,53(18)	7,4	27,9	3,3249(15)	3,7302(16)
Cg5	Cg6	[1565]	5,899(2)	26,6359	75,1(2)	44,8	77,4	1,2887(15)	4,1837(18)
Cg6	Cg3	[2655]	4,745(2)	0,0627	68,3(2)	9,4	71,7	1,4910(18)	4,6820(16)
Cg6	Cg4	[1455]	3,968(3)	17,4352	18,7(2)	27,8	25,7	3,5755(18)	3,5112(18)

[2655]	1-Y,X,1/4+Z
[1555]	X,Y,Z
[1655]	1+X,Y,Z
[1455]	-1+X,Y,Z
[1545]	X,-1+Y,Z
[4564]	Y,1-X,-1/4+Z
[4664]	1+Y,1-X,-1/4+Z
[1565]	X,1+Y,Z

Analysis of X-H...Cg(Pi-Ring) Interactions (H...Cg < 3.0 Ang. - Gamma < 40.0 Deg)

- Cg(J) = Center of gravity of ring J (Plane number above)

- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- X-H..Cg = X-H-Cg angle (degrees)
- X..Cg = Distance of X to Cg (Angstrom)
- X-H, Pi = Angle of the X-H bond with the Pi-plane (i.e. ' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C9-H9	Cg3	[1655]	2,72	-2,65	13,08	170	3,655(5)	76
C44-H44	Cg6	[4564]	2,78	2,72	12,03	136	3,525(5)	57

[1655]	1+X,Y,Z
[4564]	Y,1-X,-1/4+Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,85023(17)	0,45795(17)	0,58240(4)
Cg2	0,84335(18)	0,27987(14)	0,48419(5)
Cg3	0,75452(15)	0,50985(16)	0,39821(4)
Cg4	1,33732(15)	0,40775(16)	0,45419(5)
Cg5	0,61505(14)	1,03667(14)	0,59943(4)
Cg6	0,34238(16)	0,49530(17)	0,55540(5)

Table S7: Non-coordinative interactions in **6**.

6-Membered Ring (1) N1 --> C31 --> C32 --> C33 --> C34 --> C35 -->
 6-Membered Ring (2) N2 --> C36 --> C39A --> C40A --> C41A --> C42A -->
 6-Membered Ring (3) N2 --> C36 --> C39 --> C40 --> C41 --> C42 -->
 6-Membered Ring (4) C5 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (5) C15 --> C16 --> C17 --> C18 --> C19 --> C20 -->
 6-Membered Ring (6) C25 --> C26 --> C27 --> C28 --> C29 --> C30 -->
 6-Membered Ring (7) C34 --> C35 --> C36 --> C39A --> C38A --> C37A -->
 6-Membered Ring (8) C34 --> C35 --> C36 --> C39 --> C38 --> C37 -->

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.000 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	Cg2	[2666]	5,856(3)	-2,3357	13,1(2)	55,1	68,1	2,1806(10)	3,350(2)
Cg1	Cg5	[1555]	5,6085(15)	8,9398	77,83(12)	11	85,6	0,4306(10)	5,5061(10)
Cg1	Cg6	[1655]	5,1757(15)	-7,2835	37,67(12)	57,4	38,7	4,0421(9)	2,7904(10)
Cg2	Cg2	[2666]	3,646(3)	-2,3357	0,0(3)	43,3	43,3	2,653(2)	2,653(2)
Cg2	Cg3	[2666]	4,084(4)	-7,6254	22,7(3)	38,8	22,2	3,780(2)	3,180(2)
Cg2	Cg5	[2666]	5,752(3)	-16,0737	89,9(2)	55,3	35,4	4,686(2)	3,2719(10)
Cg3	Cg2	[2666]	4,084(4)	-2,3357	22,7(3)	22,2	38,8	3,180(2)	3,780(2)
Cg3	Cg3	[2666]	4,543(4)	-7,6254	0,0(3)	18,8	18,8	4,300(3)	4,300(3)
Cg4	Cg4	[2565]	3,8722(16)	-2,3861	0,02(13)	24,2	24,2	3,5311(11)	3,5310(11)
Cg4	Cg5	[1455]	5,9152(17)	7,4395	82,08(13)	53,4	60,5	2,9151(11)	3,5255(11)
Cg5	Cg2	[2666]	5,752(3)	-2,3357	89,9(2)	35,4	55,3	3,2719(10)	4,686(2)
Cg5	Cg3	[2666]	5,545(3)	-7,6254	67,3(2)	30,6	83	0,6740(10)	4,771(2)
Cg5	Cg4	[2665]	5,3689(15)	-10,532	82,08(13)	28,1	89,9	0,0056(11)	4,7374(11)
Cg6	Cg1	[1455]	5,1758(15)	2,0268	37,67(12)	38,7	57,4	2,7903(10)	4,0420(9)
Cg6	Cg4	[2565]	5,8181(16)	-2,3861	83,53(13)	31,2	73,5	1,6523(12)	4,9742(11)
Cg6	Cg5	[1545]	5,0121(16)	1,7133	73,05(13)	11,2	77,7	1,0718(11)	4,9164(11)

[2666]	1-X,1-Y,1-Z
[1555]	X,Y,Z
[1655]	1+X,Y,Z
[2565]	-X,1-Y,-Z
[1455]	-1+X,Y,Z
[2665]	1-X,1-Y,-Z
[1545]	X,-1+Y,Z

Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 40.0 Deg)

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- X-H..Cg = X-H-Cg angle (degrees)

- X..Cg = Distance of X to Cg (Angstrom)

- X-H, Pi = Angle of the X-H bond with the Pi-plane (i.e. ' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C16-H16	Cg6	[1565]	2,96	-2,95	5,94	142	3,756(3)	57
C40A-H40A	Cg2	[2666]	2,81	2,75	12,23	88	2,936(6)	4
[1565]	X,1+Y,Z							
[2666]	1-X,1-Y,1-Z							

Analysis of Y-X...Cg(Pi-Ring) Interactions (X..Cg < 4.0 Ang. - Gamma < 30.0 Deg)

Y--X(I)	Cg(J)	[ARU(J)]	X..Cg	X-Perp	Gamma	Y-X..Cg	Y..Cg	Y-X,Pi
C1-F1	Cg6	[1655]	3,858(2)	3,356	29,56	167,06(15)	5,167(3)	47,72
C1-F3	Cg4	[2665]	3,577(2)	3,266	24,07	102,79(15)	4,087(3)	30,24
C21-F5	Cg3	[2656]	3,995(3)	-3,699	22,18	112,99(18)	4,699(4)	18,12

[1655]	1+X,Y,Z
[2665]	1-X,1-Y,-Z
[2656]	1-X,-Y,1-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,80129(8)	0,28665(8)	0,32147(6)
Cg2	0,4759(2)	0,3597(2)	0,49575(14)
Cg3	0,4884(2)	0,3159(2)	0,50883(13)
Cg4	0,14395(11)	0,57318(8)	0,01021(6)
Cg5	0,58358(11)	0,72657(8)	0,17276(6)
Cg6	0,12228(12)	-0,00357(8)	0,16133(7)

Table S8: Non-coordinative interactions in 7.

6-Membered Ring (1) N1 --> C31 --> C32 --> C33 --> C34 --> C35 -->
 6-Membered Ring (2) N2 --> C36 --> C37 --> C38 --> C39 --> C40 -->
 6-Membered Ring (3) C5 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (4) C15 --> C16 --> C17 --> C18 --> C19 --> C20 -->
 6-Membered Ring (5) C25 --> C26 --> C27 --> C28 --> C29 --> C30 -->

Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.0 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	Cg1	[2566]	5,7078(19)	-3,197	0,04(13)	55,5	55,5	3,2347(11)	3,2347(11)
Cg1	Cg2	[2566]	3,7247(15)	-3,3423	6,01(12)	24,2	20	3,5006(11)	3,3972(10)
Cg1	Cg4	[1545]	5,8143(16)	7,0411	86,17(13)	31,3	81,2	0,8887(10)	4,9682(13)
Cg2	Cg1	[2566]	3,7247(15)	-3,197	6,01(12)	20	24,2	3,3972(10)	3,5005(11)
Cg2	Cg2	[2566]	5,5142(15)	-3,3423	0,02(12)	52,9	52,9	3,3250(10)	3,3250(10)
Cg2	Cg3	[1555]	4,7549(15)	10,6198	50,76(13)	31,3	36,3	3,8337(11)	4,0640(12)
Cg2	Cg4	[1545]	5,4088(17)	7,0411	83,36(13)	27,4	71	1,7609(11)	4,8009(13)
Cg3	Cg2	[1555]	4,7549(15)	0,0173	50,76(13)	36,3	31,3	4,0639(12)	3,8337(11)
Cg3	Cg4	[1545]	4,8758(17)	7,0411	32,61(14)	57,9	37,4	3,8735(11)	2,5942(13)
Cg3	Cg5	[1545]	5,806(2)	12,5445	19,06(14)	58	50,1	3,7223(12)	3,0724(13)
Cg4	Cg1	[2566]	5,9208(17)	-3,197	86,17(13)	43,1	64,2	2,5793(13)	4,3260(10)
Cg4	Cg3	[1565]	4,8757(17)	8,4727	32,61(14)	37,4	57,9	2,5941(13)	3,8735(11)
Cg4	Cg4	[2576]	4,0625(18)	-8,0478	0,04(14)	32,2	32,2	3,4373(12)	3,4372(12)
Cg4	Cg5	[1555]	5,9175(19)	6,7314	51,66(15)	29,9	29,6	5,1443(13)	5,1292(13)
Cg5	Cg3	[1565]	5,806(2)	8,4727	19,06(14)	50,1	58	3,0724(13)	3,7222(12)
Cg5	Cg4	[1555]	5,9176(19)	11,4851	51,66(15)	29,6	29,9	5,1293(13)	5,1444(13)

[2566]	-X,1-Y,1-Z
[1545]	X,-1+Y,Z
[1555]	X,Y,Z
[1565]	X,1+Y,Z
[2576]	-X,2-Y,1-Z

Analysis of X-H...Cg(Pi-Ring) Interactions (H...Cg < 3.0 Ang. - Gamma < 40.0 Deg)

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- X-H...Cg = X-H-Cg angle (degrees)
- X...Cg = Distance of X to Cg (Angstrom)
- X-H, Pi = Angle of the X-H bond with the Pi-plane (i.e. ' Perpendicular = 90 degrees, Parallel = 0 degrees)

X-H(I)	Cg(J)	[ARU(J)]	H...Cg	H-Perp	Gamma	X-H...Cg	X...Cg	X-H,Pi
C43-H43B	Cg3	[2667]	2,77	2,74	7,72	149	3,651(3)	64

[2667]	1-X,1-Y,2-Z
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Analysis of Y-X...Cg(Pi-Ring) Interactions (X..Cg < 4.0 Ang. - Gamma < 30.0 Deg)

Y--X(I)	Cg(J)	[ARU(J)]	X..Cg	X-Perp	Gamma	Y-X..Cg	Y..Cg	Y-X,Pi
C1-F1	Cg5	[1545]	3,510(2)	-3,105	27,8	116,43(14)	4,277(3)	30,18
C1-F3	Cg1	[1555]	3,677(2)	-3,35	24,34	123,42(15)	4,556(3)	31,86
C21-F7	Cg5	[2677]	3,396(3)	3,277	15,22	102,43(19)	3,903(4)	27,48
C21-F9	Cg5	[2677]	3,853(3)	3,518	24,06	82,15(18)	3,903(4)	16,05

[1545]	X,-1+Y,Z
[1555]	X,Y,Z
[2677]	1-X,2-Y,2-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in (I) in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,23168(11)	0,45936(8)	0,49819(6)
Cg2	-0,00410(8)	0,43605(8)	0,64580(7)
Cg3	0,12767(11)	0,28003(10)	0,87813(7)
Cg4	0,13158(12)	1,03407(10)	0,61600(8)
Cg5	0,61868(12)	1,22418(12)	0,90289(8)

Table S9: Non-coordinative interactions in **8**.

5-Membered Ring (1) N2 --> C36 --> N3 --> C42 --> C37 -->
 6-Membered Ring (2) N1 --> C31 --> C32 --> C33 --> C34 --> C35 -->
 6-Membered Ring (3) C5 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (4) C15 --> C16 --> C17 --> C18 --> C19 --> C20 -->
 6-Membered Ring (5) C25 --> C26 --> C27 --> C28 --> C29 --> C30 -->
 6-Membered Ring (6) C37 --> C38 --> C39 --> C40 --> C41 --> C42 -->
 9-Membered Ring (7) N2 --> C36 --> N3 --> C42 --> C41 --> C40 --> C39 --> C38 --> C37 -->

Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.0 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	Cg1	[2775]	4,428(2)	-18,2379	0,00(19)	46,3	46,3	3,0574(14)	3,0573(14)
Cg1	Cg2	[2775]	3,606(2)	-18,6905	7,56(18)	24,7	26,7	3,2204(14)	3,2759(14)
Cg1	Cg5	[2765]	5,025(2)	-14,3594	48,95(18)	25,7	70,4	1,6860(14)	4,5298(16)
Cg1	Cg7	[2775]	5,333(2)	-18,2348	0,89(16)	54,8	55,5	3,0169(14)	3,0773(11)
Cg2	Cg1	[2775]	3,606(2)	-18,2379	7,56(18)	26,7	24,7	3,2759(14)	3,2204(14)
Cg2	Cg4	[2675]	5,3121(19)	7,1666	83,84(16)	31,1	56,9	2,9041(12)	4,5502(15)
Cg2	Cg6	[2775]	3,714(2)	-18,1887	8,82(17)	19,9	28	3,2781(14)	3,4930(15)
Cg2	Cg7	[2775]	3,5163(19)	-18,2348	8,24(15)	16,1	20,4	3,2950(14)	3,3779(12)
Cg3	Cg4	[2676]	4,834(2)	-3,13	68,22(18)	12,6	76	1,1712(16)	4,7172(16)
Cg4	Cg2	[2675]	5,3122(19)	-12,8967	83,84(16)	56,9	31,1	4,5502(15)	2,9042(12)
Cg4	Cg3	[1555]	5,332(2)	14,5448	68,22(18)	19,4	65,7	2,1967(16)	5,0279(16)
Cg4	Cg5	[1465]	5,616(2)	11,7071	69,17(16)	41,7	88,7	0,1237(15)	4,1920(14)
Cg5	Cg1	[1555]	5,829(2)	15,1805	48,95(18)	41,9	61,6	2,7723(16)	4,3366(14)
Cg5	Cg3	[2666]	5,467(2)	-8,2196	38,5(2)	36,6	74,8	1,4342(17)	4,3915(16)
Cg5	Cg6	[1555]	4,793(2)	15,2617	48,59(18)	21,9	55,5	2,7167(16)	4,4463(15)
Cg5	Cg7	[1555]	5,157(2)	15,2161	48,71(15)	31,5	58,1	2,7270(16)	4,3958(11)
Cg6	Cg2	[2775]	3,714(2)	-18,6905	8,82(17)	28	19,9	3,4930(15)	3,2782(14)
Cg6	Cg5	[1555]	4,793(2)	11,7089	48,59(18)	55,5	21,9	4,4463(15)	2,7167(16)
Cg6	Cg5	[2765]	4,817(2)	-14,3594	48,59(18)	20,6	68,1	1,7958(15)	4,5079(16)
Cg7	Cg1	[2775]	5,333(2)	-18,2379	0,89(16)	55,5	54,8	3,0774(11)	3,0168(14)
Cg7	Cg2	[2775]	3,5164(19)	-18,6905	8,24(15)	20,4	16,1	3,3780(12)	3,2950(14)
Cg7	Cg5	[1555]	5,157(2)	11,7089	48,71(15)	58,1	31,5	4,3958(11)	2,7270(16)
Cg7	Cg5	[2765]	4,792(2)	-14,3594	48,71(15)	20,1	68,6	1,7453(11)	4,5001(16)

[2775]	2-X,2-Y,-Z	[1555]	X,Y,Z
[2765]	2-X,1-Y,-Z	[1465]	-1+X,1+Y,Z
[2675]	1-X,2-Y,-Z	[2666]	1-X,1-Y,1-Z
[2676]	1-X,2-Y,1-Z		

Analysis of X-H...Cg(Pi-Ring) Interactions (H...Cg < 3.0 Ang. - Gamma < 40.0 Deg)

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- X-H..Cg = X-H-Cg angle (degrees)
- X..Cg = Distance of X to Cg (Angstrom)
- X-H, Pi = Angle of the X-H bond with the Pi-plane (i.e. ' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C20-H20	Cg3	[2676]	2,83	2,81	6,17	139	3,597(4)	55
C29-H29	Cg1	[2765]	2,99	-2,95	8,75	141	3,776(4)	43
C43-H43C	Cg3	[2666]	2,91	-2,86	10,71	124	3,549(5)	26

[2676]	1-X,2-Y,1-Z
[2765]	2-X,1-Y,-Z
[2666]	1-X,1-Y,1-Z

Analysis of Y-X...Cg(Pi-Ring) Interactions (X..Cg < 4.0 Ang. - Gamma < 30.0 Deg)

Y--X(I)	Cg(J)	[ARU(J)]	X..Cg	X-Perp	Gamma	Y-X..Cg	Y..Cg	Y-X,Pi
C11-F4	Cg5	[1565]	3,856(3)	-3,429	27,22	110,42(17)	4,497(4)	12,99
C21-F9	Cg2	[1555]	3,799(3)	-3,646	16,32	123,0(2)	4,663(5)	28,82
C21-F9	Cg4	[2675]	3,399(2)	-3,307	13,39	132,1(2)	4,407(4)	45,26

[1565]	X,1+Y,Z
[1555]	X,Y,Z
[2675]	1-X,2-Y,-Z

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	1,01532(12)	0,83024(10)	0,01112(9)
Cg2	0,74595(12)	1,05598(11)	-0,05983(8)
Cg3	0,51635(13)	0,67542(13)	0,63512(12)
Cg4	0,31042(12)	1,01728(12)	0,36538(8)
Cg5	0,96477(12)	0,36308(12)	0,21125(10)
Cg6	1,15397(12)	0,70085(12)	0,04710(9)
Cg7	1,09389(9)	0,75657(9)	0,03159(7)

Table S10: Non-coordinative interactions in **9**.

6-Membered Ring (1) N1 --> C1 --> C2 --> C3 --> C4 --> C5 -->
 6-Membered Ring (2) N2 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (3) C17 --> C18 --> C19 --> C20 --> C21 --> C22 -->
 6-Membered Ring (4) C27 --> C28 --> C29 --> C30 --> C31 --> C32 -->
 6-Membered Ring (5) C37 --> C38 --> C39 --> C40 --> C41 --> C42 -->#

Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.0 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	Cg3	[1555]	5,041(3)	4,1526	75,6(3)	5,3	76,6	1,1671(18)	5,020(3)
Cg1	Cg5	[3666]	4,795(3)	0,4093	83,4(2)	5,6	83,5	0,5461(18)	4,773(2)
Cg2	Cg4	[4464]	4,706(3)	-15,6374	49,7(2)	26,8	24,1	4,2977(17)	4,203(2)
Cg2	Cg5	[3666]	5,876(3)	0,4093	81,7(2)	32,7	85,7	0,4434(17)	4,943(2)
Cg3	Cg4	[2656]	5,071(3)	18,9973	60,1(3)	51,9	8,8	5,011(3)	3,131(2)
Cg3	Cg4	[4464]	4,731(3)	-15,6374	60,1(3)	18,1	69,6	1,651(3)	4,497(2)
Cg4	Cg2	[4565]	4,706(3)	-10,9702	49,7(2)	24,1	26,8	4,203(2)	4,2977(17)
Cg4	Cg3	[2646]	5,072(3)	-11,0434	60,1(3)	8,8	51,9	3,131(2)	5,012(3)
Cg4	Cg4	[3767]	4,967(3)	-16,9276	0,0(2)	47,4	47,4	3,360(2)	3,360(2)
Cg5	Cg3	[2646]	5,560(3)	-11,0434	61,7(3)	28,4	80,1	0,953(2)	4,890(3)
Cg5	Cg5	[3666]	3,754(3)	0,4093	0,0(3)	19,3	19,3	3,543(2)	3,543(2)

[1555]	X,Y,Z
[3666]	1-X,1-Y,1-Z
[4464]	-1/2+X,3/2-Y,-1/2+Z
[2656]	3/2-X,1/2+Y,3/2-Z
[4565]	1/2+X,3/2-Y,1/2+Z
[2646]	3/2-X,-1/2+Y,3/2-Z
[3767]	2-X,1-Y,2-Z

Analysis of X-H...Cg(Pi-Ring) Interactions (H..Cg < 3.0 Ang. - Gamma < 40.0 Deg)

- Cg(J) = Center of gravity of ring J (Plane number above)
- H-Perp = Perpendicular distance of H to ring plane J
- Gamma = Angle between Cg-H vector and ring J normal
- X-H..Cg = X-H-Cg angle (degrees)
- X..Cg = Distance of X to Cg (Angstrom)
- X-H, Pi = Angle of the X-H bond with the Pi-plane (i.e. ' Perpendicular = 90 degrees, Parallel = 0 degrees)

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	H-Perp	Gamma	X-H..Cg	X..Cg	X-H,Pi
C22-H22	Cg1	[1555]	2,84	2,78	12,08	154	3,721(6)	74
C28-H28	Cg3	[4565]	2,8	-2,78	6,8	134	3,526(5)	47
C39-H39	Cg1	[3666]	2,53	-2,51	5,85	165	3,450(5)	78

[1555]	X,Y,Z
[4565]	$1/2+X, 3/2-Y, 1/2+Z$
[3666]	$1-X, 1-Y, 1-Z$

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in (I) in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,42712(16)	0,70649(7)	0,55013(12)
Cg2	0,73730(15)	0,74206(7)	0,45353(12)
Cg3	0,4851(2)	0,88980(10)	0,70805(17)
Cg4	1,13923(19)	0,56914(8)	0,95723(15)
Cg5	0,5539(2)	0,46217(8)	0,60752(15)

Table S11: Non-coordinative interactions in **10**.

6-Membered Ring (1) C5 --> C6 --> C7 --> C8 --> C9 --> C10 -->
 6-Membered Ring (2) C15 --> C16 --> C17 --> C18 --> C19 --> C20 -->
 6-Membered Ring (3) C25 --> C26 --> C27 --> C28 --> C29 --> C30 -->
 6-Membered Ring (4) C35 --> C36 --> C37 --> C38 --> C39 --> C40 -->
 6-Membered Ring (5) N1 --> C41 --> C42 --> C43 --> C44 --> C45 -->

Analysis of Short Ring-Interactions with Cg-Cg Distances < 6.0 Ang., Alpha < 20.0 Deg. and Beta < 60.0 Deg.

- Cg(I) = Plane number I (= ring number in () above)
- Alpha = Dihedral Angle between Planes I and J (Deg)
- Beta = Angle Cg(I)-->Cg(J) or Cg(I)-->Me vector and normal to plane I (Deg)
- Gamma = Angle Cg(I)-->Cg(J) vector and normal to plane J (Deg)
- Cg-Cg = Distance between ring Centroids (Ang.)
- CgI_Perp = Perpendicular distance of Cg(I) on ring J (Ang.)
- CgJ_Perp = Perpendicular distance of Cg(J) on ring I (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	Cg3	[4565]	4,818(3)	-14,3655	16,3(2)	52,6	36,4	3,876(2)	2,9251(17)
Cg2	Cg1	[3766]	5,541(3)	-9,4776	47,9(2)	35,9	81,3	0,8364(17)	4,490(2)
Cg2	Cg3	[2645]	5,034(2)	2,968	59,8(2)	21,1	47,7	3,3880(18)	4,6981(18)
Cg2	Cg4	[4564]	5,810(2)	8,2752	75,2(2)	43,6	61,6	2,7622(17)	4,2111(18)
Cg2	Cg5	[1655]	3,813(3)	15,832	7,6(2)	19,5	16,5	3,6551(18)	3,594(2)
Cg3	Cg1	[4464]	4,819(3)	-19,0496	16,3(2)	36,4	52,6	2,9251(18)	3,876(2)
Cg3	Cg2	[2655]	5,034(2)	19,3611	59,8(2)	47,7	21,1	4,6983(18)	3,3881(18)
Cg3	Cg4	[4464]	5,103(2)	7,4097	71,7(2)	51,4	20,5	4,7787(17)	3,1869(18)
Cg3	Cg5	[1555]	3,741(3)	12,6296	7,1(2)	21,9	21,9	3,4710(18)	3,472(2)
Cg4	Cg2	[2655]	5,046(2)	19,3611	75,2(2)	15,3	73,5	1,4353(18)	4,8675(17)
Cg4	Cg3	[4565]	5,103(2)	-14,3655	71,7(2)	20,5	51,4	3,1872(18)	4,7786(17)
Cg4	Cg5	[4565]	5,310(3)	-19,0286	69,9(2)	23	87,9	0,1918(18)	4,888(2)
Cg5	Cg2	[1455]	3,813(3)	7,9922	7,6(2)	16,5	19,5	3,594(2)	3,6552(18)
Cg5	Cg3	[1555]	3,741(3)	15,5427	7,1(2)	21,9	21,9	3,472(2)	3,4709(18)

[4565]	1/2+X,3/2-Y,1/2+Z	[2655]	3/2-X,1/2+Y,1/2-Z
[3766]	2-X,1-Y,1-Z	[1555]	X,Y,Z
[2645]	3/2-X,-1/2+Y,1/2-Z	[4565]	1/2+X,3/2-Y,1/2+Z
[4564]	1/2+X,3/2-Y,-1/2+Z	[1455]	-1+X,Y,Z
[1655]	1+X,Y,Z	[1555]	X,Y,Z
[4464]	-1/2+X,3/2-Y,-1/2+Z		

The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	1,1673(2)	0,59895(9)	0,59492(12)
Cg2	1,1466(2)	0,50522(8)	0,25683(10)
Cg3	0,3081(2)	0,79435(8)	0,12923(10)
Cg4	0,6145(2)	0,88926(8)	0,46778(8)
Cg5	0,2881(3)	0,66441(8)	0,25540(12)

Table S12. Crystallographic data and processing parameters of **1 – 10**.

Compound	1	2	3
Empirical formula	C ₃₀ H ₂₂ F ₉ LaO ₈	C ₄₂ H ₃₀ F ₉ LaN ₂ O ₈	C ₅₄ H ₄₂ F ₉ LaN ₄ O ₆
Formula mass	820.38	1000.59	1152.82
System	Orthorhombic	Orthorhombic	Triclinic
Space group	P 2 ₁ 2 ₁ 2 ₁	P b c a	P-1
a (Å)	10.8339(3)	20.2785(8)	11.6736(4)
b (Å)	12.9651(4)	17.0836(7)	12.4587(5)
c (Å)	23.2814(8)	22.9223(10)	18.7838(8)
α (°)	90	90	93.397(2)
β (°)	90	90	95.696(2)
γ (°)	90	90	113.695(2)
V (Å ³)	3270.17(18)	8117.2(6)	2474.44(17)
Z	4	8	2
T (K)	200(2)	100(2)	100(2)
μ (mm ⁻¹)	1.404	1.150	0.952
D _{calc} (Mg/m ³)	1.666	1.638	1.547
θ max (°)	30.115	30.014	27.908
Data collected	214806	245048	128758
Unique refl. / R _{int}	9556 / 0.0318	11824 / 0.0280	11964 / 0.0478
Parameters / Restraints	465 / 1	599 / 48	671 / 0
Goodness-of-Fit on F ²	1.225	1.053	1.041
R1 / wR2 (all data)	0.0302 / 0.0534	0.0263 / 0.0601	0.0313 / 0.0749
Residual extrema (e/Å ³)	1.801 / -1.383	0.567 / -0.449	1.394 / -1.565

Table S12. Cont.

Compound	4	5	6
Empirical formula	C ₅₄ H ₄₂ F ₉ LaN ₄ O ₆	C ₄₅ H ₂₉ F ₉ LaN ₃ O ₆	C ₄₄ H ₃₂ F ₉ LaN ₂ O ₇
Formula mass	1152.83	1017.62	1010.62
System	Monoclinic	Tetragonal	Triclinic
Space group	P2 ₁ /c	P ₄ ₁	P-1
a (Å)	14.2828(5)	10.5985(3)	10.0568(8)
b (Å)	23.0917(9)	10.5985(3)	12.3260(10)
c (Å)	15.3962(6)	38.1184(12)	17.9092(14)
α (°)	90	90	77.756(5)
β (°)	99.060(2)	90	79.585(5)
γ (°)	90	90	75.818(5)
V (Å ³)	5014.5(3)	4281.8(3)	2083.9(3)
Z	4	4	2
T (K)	100(2)	100(2)	100(2)
μ (mm ⁻¹)	0.940	1.089	1.119
D _{calc} (Mg/m ³)	1.527	1.579	1.611
θ max (°)	27.999	33.162	33.175
Data collected	12101	16324	15742
Unique refl. / R _{int}	8659 / 0.1097	15859 / 0.0833	11445 / 0.0903
Parameters / Restraints	690 / 12	578 / 1	650 / 42
Goodness-of-Fit on F ²	1.012	1.249	1.013
R1 / wR2 (all data)	0.0338 / 0.0694	0.0353 / 0.0740	0.0442 / 0.0850
Residual extrema (e/Å ³)	0.832 / -0.842	1.015 / -2.032	1.015 / -2.032

Table S12. cont.

Compound	7	8
Empirical formula	C ₄₄ H ₃₆ F ₉ LaN ₂ O ₇	C ₄₃ H ₃₁ F ₉ LaN ₃ O ₇
Formula mass	1014.66	1011.62
System	Triclinic	Triclinic
Space group	P-1	P-1
a (Å)	11.5915(4)	11.2215(14)
b (Å)	11.9970(4)	13.5211(16)
c (Å)	17.0947(6)	15.2503(19)
α (°)	101.329(2)	65.583(6)
β (°)	106.027(2)	78.991(7)
γ (°)	104.460(2)	81.622(6)
V (Å ³)	2120.61(13)	2062.4(5)
Z	2	2
T (K)	100(2)	100(2)
μ (mm ⁻¹)	1.100	1.131
D _{calc} (Mg/m ³)	1.589	1.629
θ max (°)	30.238	26.999
Data collected	85423	59257
Unique refl. / R _{int}	12494 / 0.0369	8988 / 0.0592
Parameters / Restraints	574 / 9	572 / 3
Goodness-of-Fit on F ²	1.099	1.042
R1 / wR2 (all data)	0.0368 / 0.849	0.0379 / 0.0827
Residual extrema (e/Å ³)	1.225 / -1.533	1.439 / -1.565

Table S12. cont.

Compound	9	10
Empirical formula	C ₄₂ H ₃₀ F ₉ N ₂ O ₆ Tb	C ₄₅ H ₃₀ EuF ₁₂ NO ₈
Formula mass	988.60	1092.66
System	Monoclinic	Monoclinic
Space group	P2 ₁ /n	P2 ₁ /n
a (Å)	11.1935(4)	11.1009(6)
b (Å)	24.2208(7)	21.8025(12)
c (Å)	15.5561(5)	18.7796(11)
α (°)	90	90
β (°)	103.7180(10)	106.930(3)
γ (°)	90	90
V (Å ³)	4097.2(2)	4348.2(4)
Z	4	4
T (K)	100(2)	100(2)
μ (mm ⁻¹)	1.816	1.549
D _{calc} (Mg/m ³)	1.603	1.669
θ max (°)	23.857	27.532
Data collected	79220	20270
Unique refl. / R _{int}	6314 / 0.0151	8405 / 0.1708
Parameters / Restraints	547 / 21	484 / 7
Goodness-of-Fit on F ²	1.144	1.012
R1 / wR2 (all data)	0.0323 / 0.0736	0.0702 / 0.1476
Residual extrema (e/Å ³)	1.250 / -1.358	1.424 / -1.055

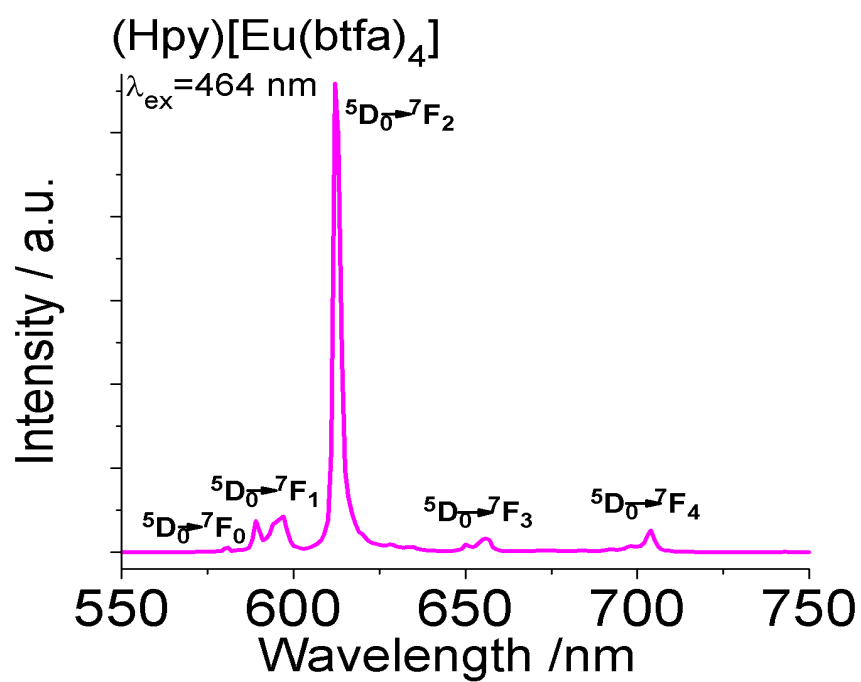


Figure S21: Emission spectrum of **10** measured at the 464 nm excitation wavelength.