

ELECTRONIC SUPPLEMENTARY INFORMATION (ESI)

Slow magnetic relaxation and luminescence properties in neodymium(III)-4,4,4-trifluoro-1-(2-naphthyl)butane-1,3- dionato complexes incorporating bipyridyl ligands†

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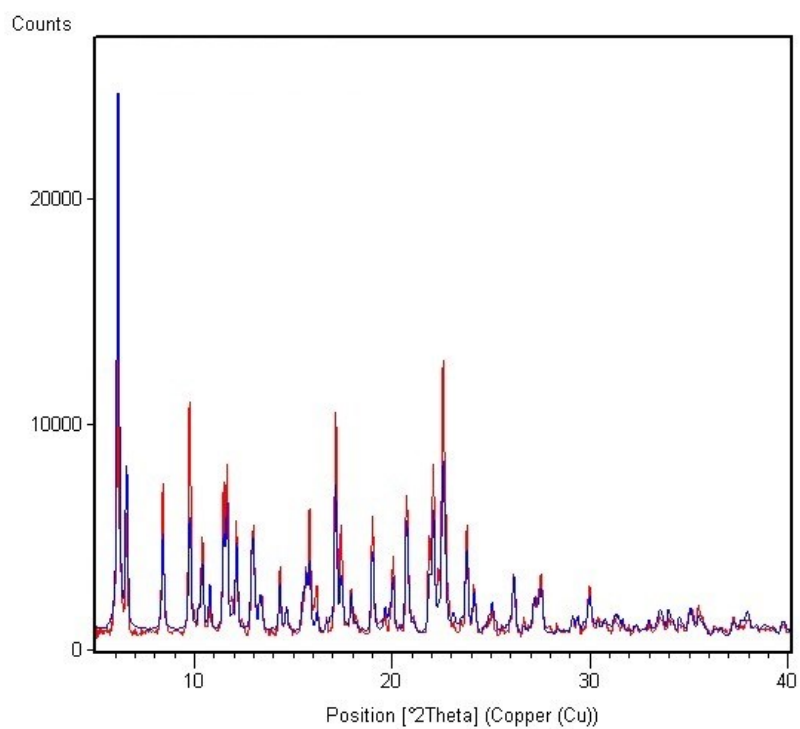


Fig. S1 Observed (red) and simulated (blue) PXRD of **1**.

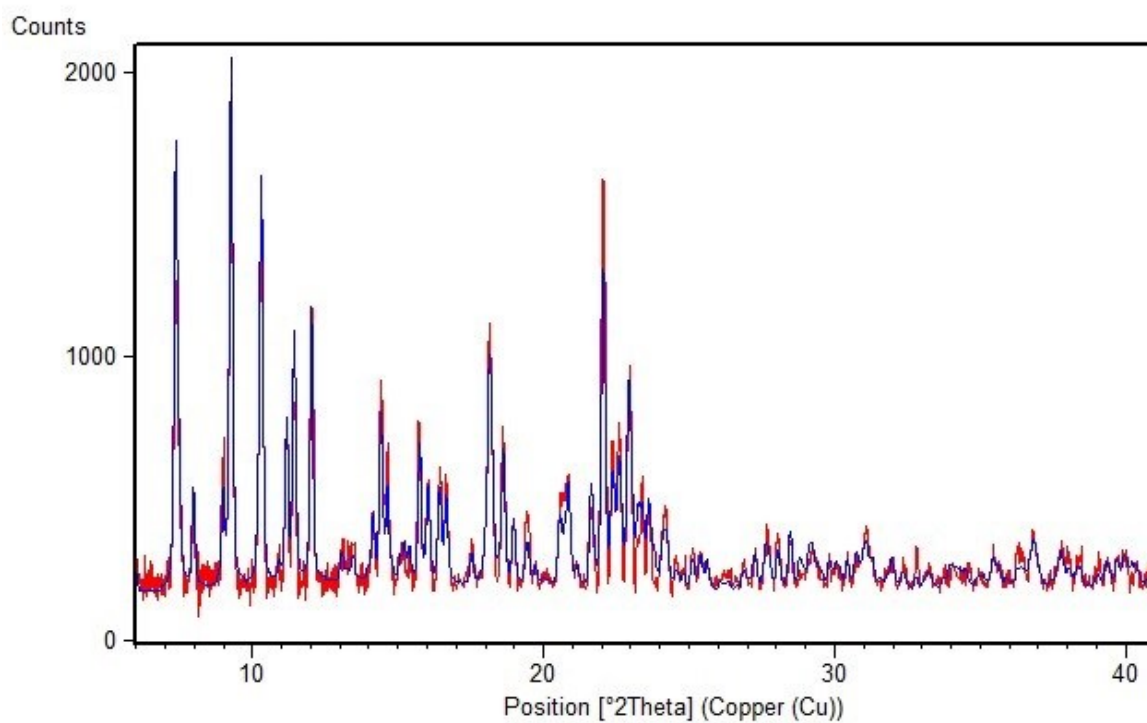


Fig. S2 Observed (red) and simulated (blue) PXRD of **2**.

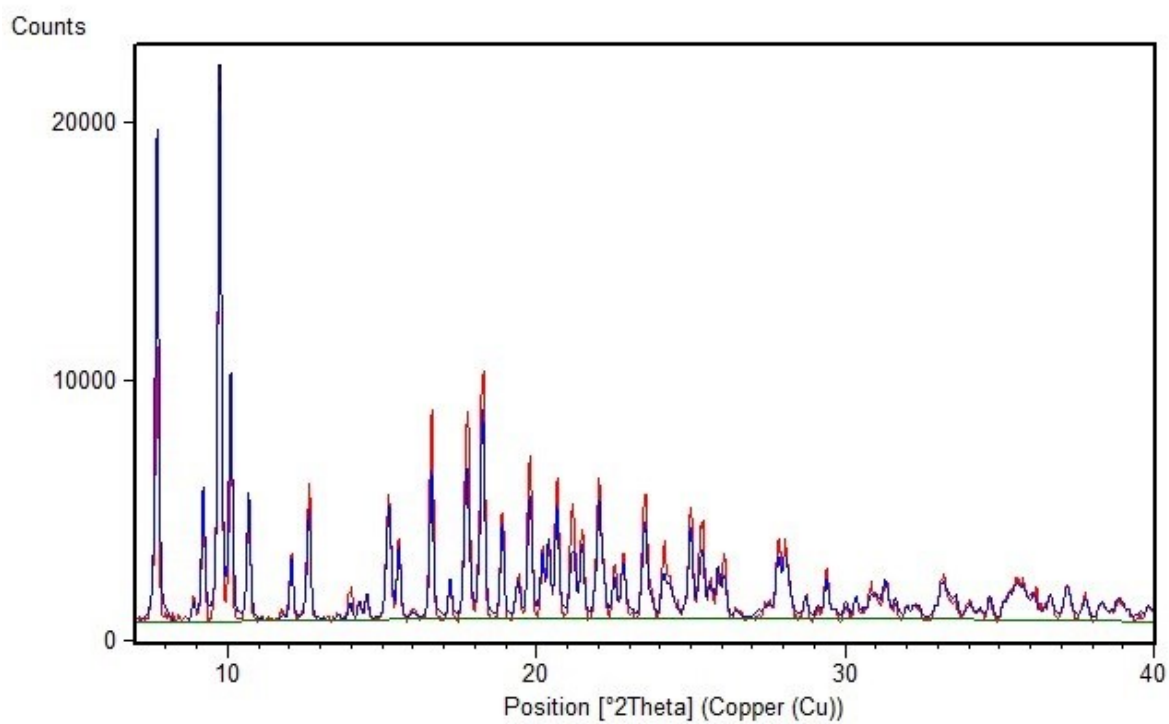


Fig. S3 Observed (red) and simulated (blue) PXR D of **3**.

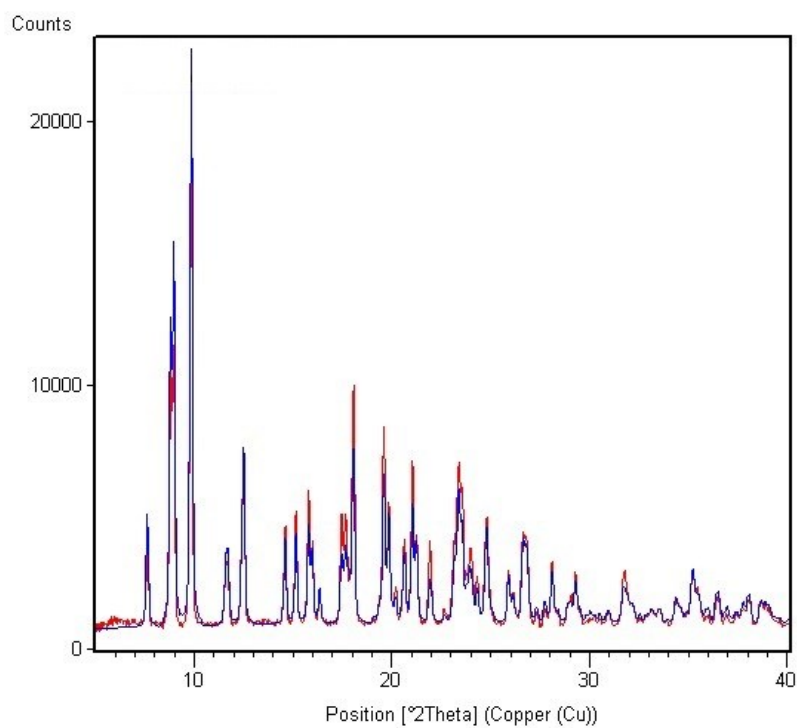


Fig. S4 Observed (red) and simulated (blue) PXR D of **4**.

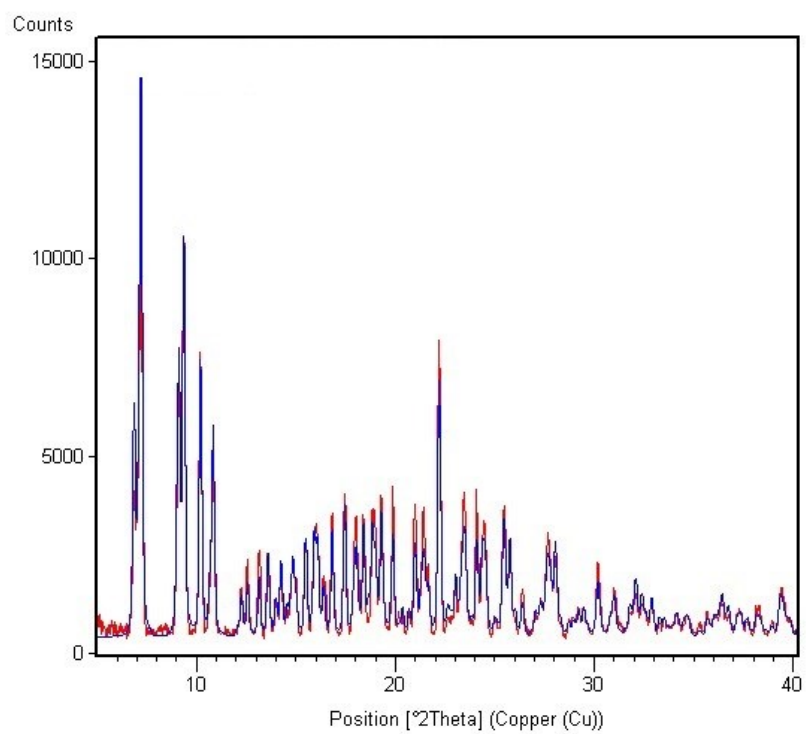


Fig. S5 Observed (red) and simulated (blue) PXRD of **5**.

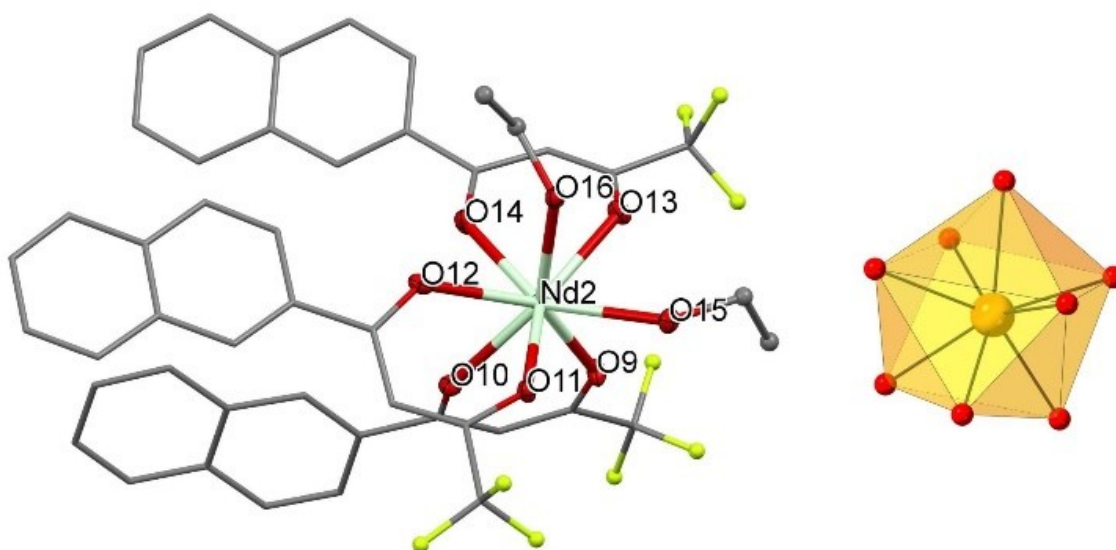


Fig. S6 Perspective view of Nd2 polyhedron (left) and coordination figure (right) of **1**.

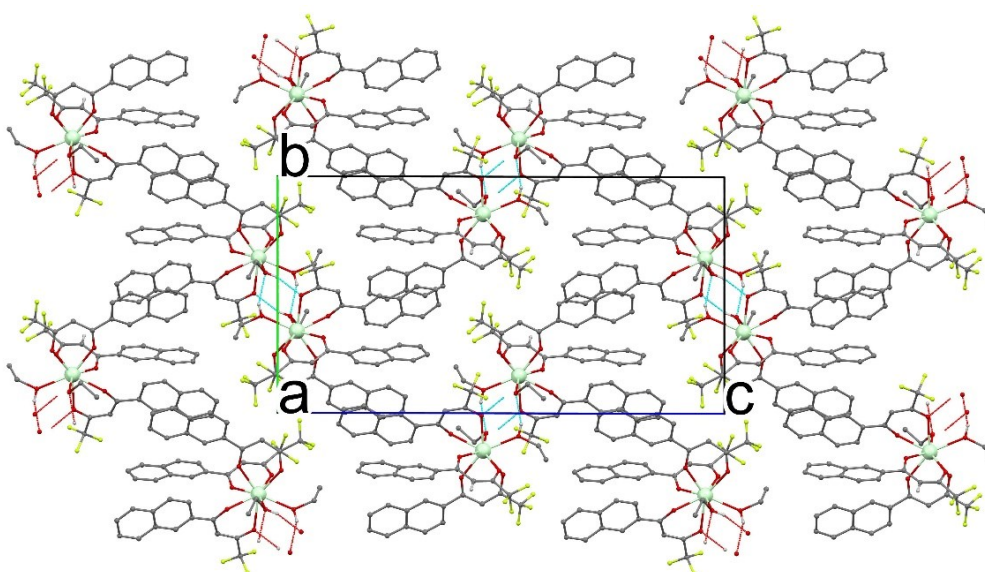


Fig. S7 Packing plot of **1**.

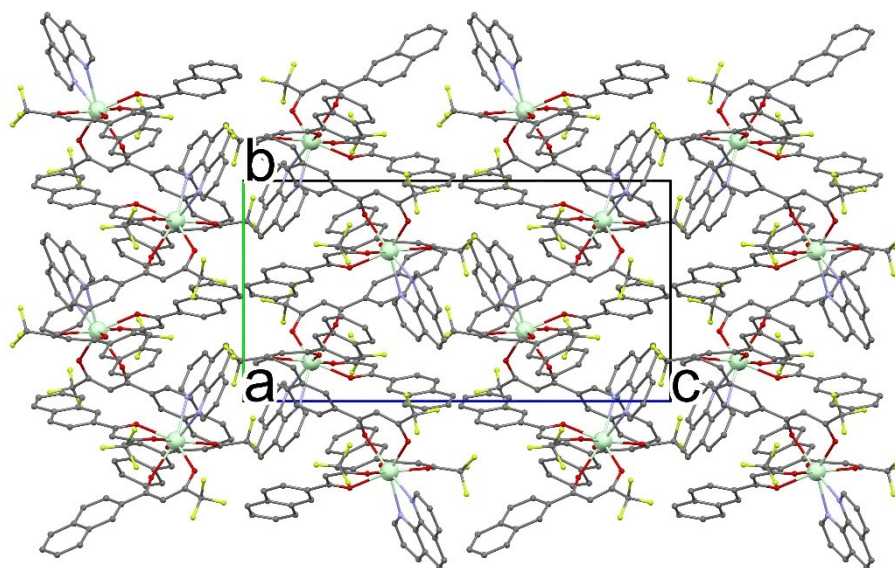


Fig. S8 Packing plot of **2**.

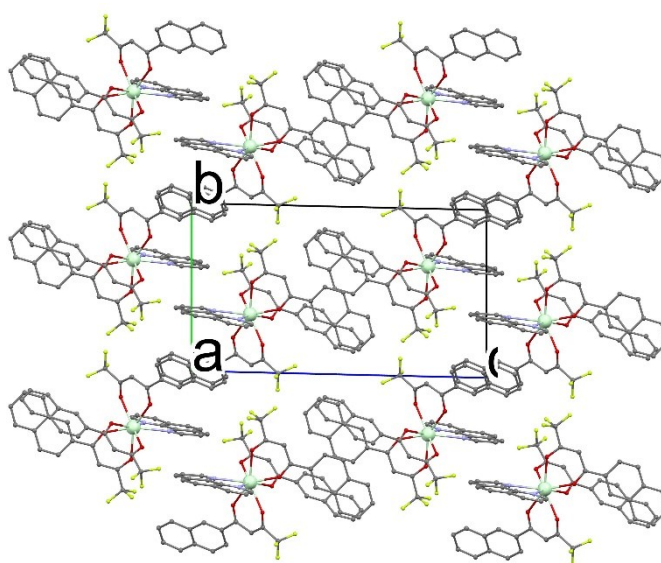


Fig. S9 Packing plot of **2a**.

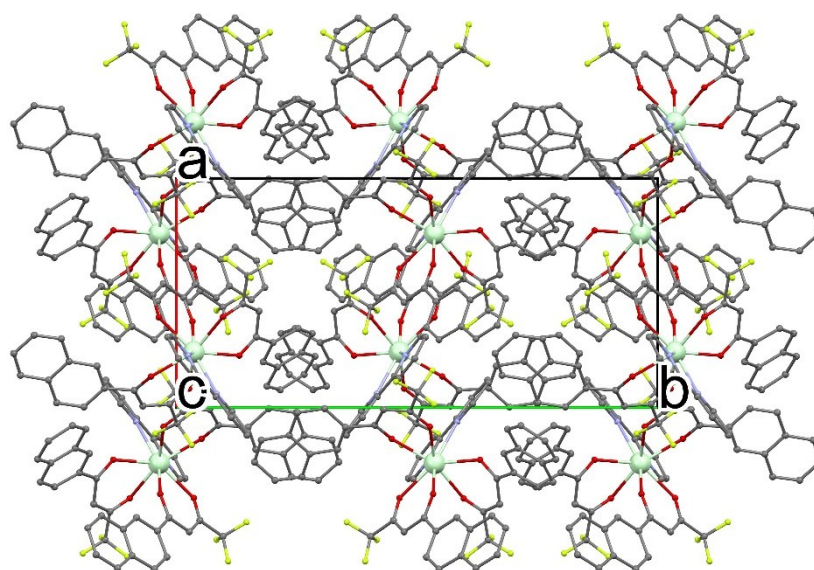


Fig. S10 Packing plot of **3**.

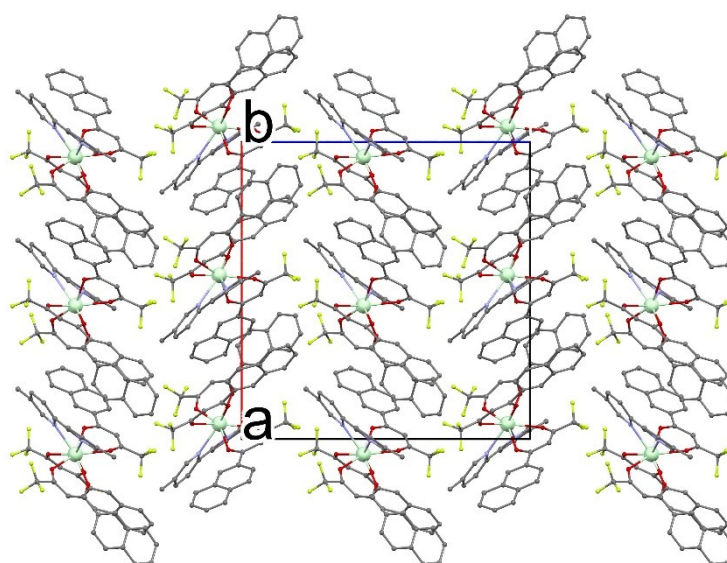


Fig. S11 Packing plot of **4**.

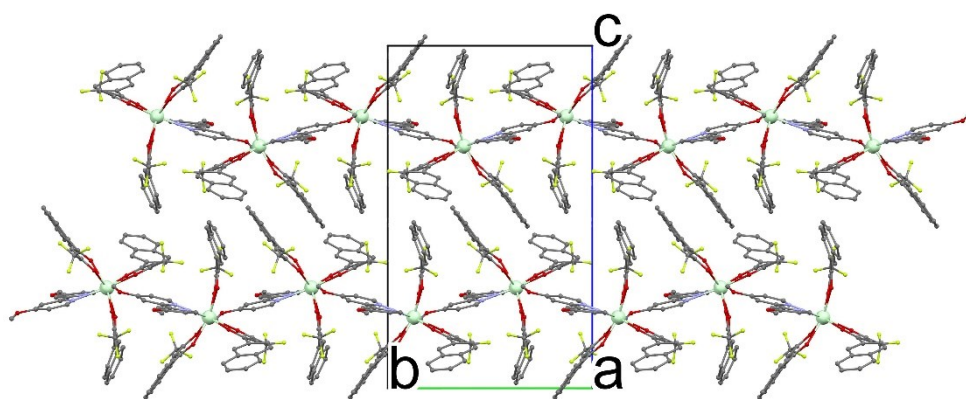


Fig. S12 Packing plot of **5**.

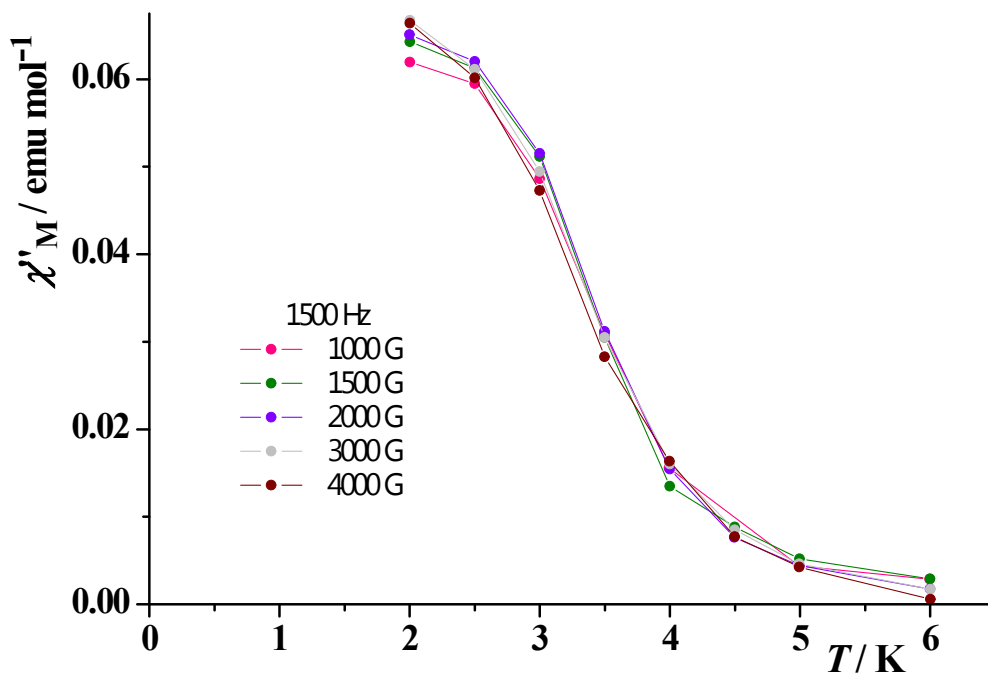


Fig. S13 χ_M'' versus T values at dc fields up to 0.4 T of **3**. Oscillating ac field of 4×10^{-4} T at 1488 Hz.

Table S1. Continuous shape measures (CShM's) using SHAPE software for compounds **2-5**.

		2	2a	3	4	5
TDD-8	D _{2d}	2.094	2.389	1.294	2.309	0.815
SAPR-8	D _{4d}	0.826	0.921	1.391	0.849	3.362
BTPR-8	C _{2v}	2.584	2.482	1.690	1.967	2.662
JBTPR-8	C _{2v}	3.135	2.973	2.265	2.525	3.399

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

6-Membered Ring (1)	C5	-->	C6	-->	C7	-->	C12	-->	C13	-->	C14	-->								
6-Membered Ring (2)	C7	-->	C8	-->	C9	-->	C10	-->	C11	-->	C12	-->								
6-Membered Ring (3)	C19	-->	C20	-->	C21	-->	C26	-->	C27	-->	C28	-->								
6-Membered Ring (4)	C21	-->	C22	-->	C23	-->	C24	-->	C25	-->	C26	-->								
6-Membered Ring (5)	C33	-->	C34	-->	C35	-->	C40	-->	C41	-->	C42	-->								
6-Membered Ring (6)	C35	-->	C36	-->	C37	-->	C38	-->	C39	-->	C40	-->								
10-Membered Ring (7)	C5	-->	C6	-->	C7	-->	C8	-->	C9	-->	C10	-->	C11	-->	C12	-->	C13	-->	C14	-->
10-Membered Ring (8)	C19	-->	C20	-->	C21	-->	C22	-->	C23	-->	C24	-->	C25	-->	C26	-->	C27	-->	C28	-->
10-Membered Ring (9)	C33	-->	C34	-->	C35	-->	C36	-->	C37	-->	C38	-->	C39	-->	C40	-->	C41	-->	C42	-->
6-Membered Ring (10)	C51	-->	C52	-->	C53	-->	C58	-->	C59	-->	C60	-->								
6-Membered Ring (11)	C53	-->	C54	-->	C55	-->	C56	-->	C57	-->	C58	-->								
6-Membered Ring (12)	C65	-->	C66	-->	C67	-->	C68	-->	C73	-->	C74	-->								
6-Membered Ring (13)	C68	-->	C69	-->	C70	-->	C71	-->	C72	-->	C73	-->								
6-Membered Ring (14)	C79	-->	C80	-->	C81	-->	C86	-->	C87	-->	C88	-->								
6-Membered Ring (15)	C81	-->	C82	-->	C83	-->	C84	-->	C85	-->	C86	-->								
10-Membered Ring (16)	C51	-->	C52	-->	C53	-->	C54	-->	C55	-->	C56	-->	C57	-->	C58	-->	C59	-->	C60	-->
10-Membered Ring (17)	C65	-->	C66	-->	C67	-->	C68	-->	C69	-->	C70	-->	C71	-->	C72	-->	C73	-->	C74	-->
10-Membered Ring (18)	C79	-->	C80	-->	C81	-->	C82	-->	C83	-->	C84	-->	C85	-->	C86	-->	C87	-->	C88	-->

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.)
- Slippage = Distance between Cg(I) and Perpendicular Projection 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	[1655]	4,639(3)	6,3327	66,5(3)	5,9	71,2	1,495(2)	4,614(2)
Cg1	Cg6	[1655]	5,887(3)	6,2591	66,7(3)	21	75,5	1,473(2)	5,495(2)
Cg1	Cg9	[1655]	5,157(3)	6,2822	66,6(2)	11,4	73,3	1,486(2)	5,0556(18)
Cg1	Cg12	[2666]	5,049(3)	-8,165	1,8(3)	45,9	47,6	3,406(2)	3,516(3)
Cg1	Cg13	[2666]	3,873(4)	-8,2075	1,6(3)	27,2	28,4	3,407(2)	3,445(3)
Cg1	Cg13	[2766]	5,991(4)	-14,8359	1,6(3)	57	57,5	3,222(2)	3,260(3)
Cg1	Cg17	[2666]	4,332(3)	-8,1772	1,7(2)	36,5	38,1	3,408(2)	3,481(2)
Cg2	Cg5	[1655]	5,345(3)	6,3327	65,0(3)	30,1	71,4	1,703(2)	4,624(2)
Cg2	Cg6	[1655]	5,525(4)	6,2591	65,2(3)	8,2	72,3	1,679(2)	5,468(2)
Cg2	Cg9	[1655]	5,297(3)	6,2822	65,1(2)	17,7	71,4	1,690(2)	5,0471(18)
Cg2	Cg12	[2666]	3,822(4)	-8,165	2,9(3)	22,9	23,7	3,498(3)	3,521(3)
Cg2	Cg13	[2666]	3,989(4)	-8,2075	2,6(3)	31,4	29	3,490(3)	3,406(3)
Cg2	Cg17	[2666]	3,711(3)	-8,1772	2,8(2)	21	19,5	3,497(3)	3,464(2)
Cg3	Cg5	[1555]	5,370(3)	9,4061	64,7(3)	22,6	77,2	1,193(2)	4,958(2)
Cg3	Cg6	[1555]	4,873(4)	9,3644	65,0(3)	13,3	76	1,182(2)	4,743(2)
Cg3	Cg7	[1555]	5,978(3)	12,0198	15,6(2)	58,9	57,3	3,231(3)	3,086(2)
Cg3	Cg9	[1555]	4,978(3)	9,3727	64,9(2)	13	76,2	1,187(2)	4,8494(18)

Cg3	Cg14	[2676]	4,855(3)	-20,8219	2,3(3)	45,8	43,8	3,504(3)	3,382(2)
Cg3	Cg15	[2676]	3,773(4)	-20,8087	3,4(3)	22,1	21,6	3,508(3)	3,495(3)
Cg3	Cg18	[2676]	4,174(3)	-20,8264	2,8(2)	34,5	32,6	3,517(3)	3,4411(19)
Cg4	Cg6	[1555]	5,027(4)	9,3644	64,3(3)	19,3	70,1	1,712(3)	4,743(2)
Cg4	Cg9	[1555]	5,659(3)	9,3727	64,2(2)	30,5	72,3	1,720(3)	4,8751(18)
Cg4	Cg14	[2676]	3,796(4)	-20,8219	1,0(3)	25,7	25,1	3,438(3)	3,421(2)
Cg4	Cg15	[2676]	4,121(4)	-20,8087	1,9(3)	32,4	34,3	3,404(3)	3,477(3)
Cg4	Cg18	[2676]	3,771(3)	-20,8264	1,4(3)	23,7	24,4	3,433(3)	3,4515(19)
Cg5	Cg3	[1455]	5,906(3)	10,8346	64,7(3)	43,7	72,9	1,737(2)	4,266(2)
Cg5	Cg12	[2666]	5,695(3)	-8,165	66,6(3)	20,5	76,2	1,358(2)	5,334(3)
Cg5	Cg13	[2666]	4,807(3)	-8,2075	66,3(3)	9,4	73,3	1,383(2)	4,742(3)
Cg5	Cg15	[2576]	5,277(3)	-14,2909	63,0(3)	23,6	67,7	1,998(2)	4,835(2)
Cg5	Cg17	[2666]	5,125(3)	-8,1772	66,5(2)	10,6	74,5	1,372(2)	5,037(2)
Cg5	Cg18	[2576]	5,975(3)	-14,2406	63,6(2)	33,9	71	1,942(2)	4,9598(18)
Cg6	Cg12	[2666]	5,348(3)	-8,165	66,8(3)	4,9	64,4	2,309(2)	5,328(3)
Cg6	Cg13	[2666]	5,502(3)	-8,2075	66,5(3)	30,6	65	2,324(2)	4,738(3)
Cg6	Cg14	[2576]	5,558(3)	-14,1779	64,3(3)	23,6	73,7	1,564(2)	5,094(2)
Cg6	Cg15	[2576]	4,887(3)	-14,2909	63,2(3)	7,8	70,1	1,665(2)	4,843(2)
Cg6	Cg17	[2666]	5,285(3)	-8,1772	66,7(2)	17,8	64	2,320(2)	5,032(2)
Cg6	Cg18	[2576]	5,088(3)	-14,2406	63,8(2)	12,5	71,4	1,621(2)	4,9682(18)
Cg7	Cg3	[1555]	5,978(3)	17,5291	15,6(2)	57,3	58,9	3,0863(19)	3,231(3)
Cg7	Cg5	[1655]	4,851(3)	6,3327	65,8(2)	18,2	70,8	1,5977(18)	4,609(2)
Cg7	Cg6	[1655]	5,574(3)	6,2591	66,0(2)	11	73,6	1,5746(18)	5,472(2)
Cg7	Cg9	[1655]	5,081(3)	6,2822	65,84(17)	7,1	71,8	1,5869(18)	5,0416(18)
Cg7	Cg12	[2666]	4,309(3)	-8,165	2,3(2)	35	36,7	3,4541(19)	3,529(3)
Cg7	Cg13	[2666]	3,738(3)	-8,2075	2,0(2)	23,2	22,6	3,4502(19)	3,437(3)
Cg7	Cg17	[2666]	3,845(3)	-8,1772	2,15(18)	25,1	26	3,4547(19)	3,483(2)
Cg8	Cg5	[1555]	5,812(3)	9,4061	64,4(2)	31,2	75,5	1,4569(19)	4,969(2)
Cg8	Cg6	[1555]	4,794(3)	9,3644	64,6(2)	9,6	72,4	1,4464(19)	4,726(2)
Cg8	Cg9	[1555]	5,184(3)	9,3727	64,51(17)	20,8	73,7	1,4531(19)	4,8462(18)
Cg8	Cg14	[2676]	4,185(3)	-20,8219	1,6(2)	35,2	33,9	3,474(2)	3,421(2)
Cg8	Cg15	[2676]	3,759(3)	-20,8087	2,6(2)	21,3	23,1	3,459(2)	3,504(3)
Cg8	Cg18	[2676]	3,788(3)	-20,8264	2,03(18)	23,8	23,3	3,478(2)	3,4648(19)
Cg9	Cg3	[1455]	5,889(3)	10,8346	64,9(2)	43,4	71,7	1,8451(18)	4,278(2)
Cg9	Cg12	[2666]	5,387(3)	-8,165	66,7(2)	8,3	70,1	1,8334(18)	5,330(3)
Cg9	Cg13	[2666]	5,018(3)	-8,2075	66,4(2)	19,1	68,3	1,8537(18)	4,742(3)
Cg9	Cg15	[2576]	4,937(3)	-14,2909	63,1(2)	11,4	68,2	1,8308(18)	4,840(2)
Cg9	Cg17	[2666]	5,059(3)	-8,1772	66,55(17)	5,6	68,6	1,8463(18)	5,035(2)
Cg9	Cg18	[2576]	5,413(3)	-14,2406	63,73(17)	23,4	70,8	1,7812(18)	4,9672(18)
Cg10	Cg2	[2766]	5,056(3)	-11,2381	68,2(3)	11,5	66,1	2,051(2)	4,954(2)
Cg10	Cg3	[2676]	5,598(3)	-20,8761	67,8(3)	20,1	76,2	1,338(2)	5,257(2)
Cg10	Cg4	[2676]	4,809(3)	-20,4682	67,1(3)	8,9	72,9	1,410(2)	4,751(3)
Cg10	Cg7	[2766]	5,523(3)	-11,1186	68,9(2)	23,6	68,9	1,988(2)	5,0609(19)
Cg10	Cg8	[2676]	5,073(3)	-20,6762	67,4(2)	9,5	74,1	1,393(2)	5,0040(19)
Cg10	Cg12	[1655]	5,734(3)	13,7408	69,8(3)	36,7	73,6	1,616(2)	4,598(3)

Cg11	Cg1	[2766]	5,226(3)	-11,0246	68,9(3)	13,2	71,7	1,644(2)	5,087(2)
Cg11	Cg2	[2766]	5,122(3)	-11,2381	67,5(3)	14,3	69,9	1,761(2)	4,963(2)
Cg11	Cg3	[2676]	5,321(3)	-20,8761	67,7(3)	7,6	65	2,249(2)	5,275(2)
Cg11	Cg4	[2676]	5,586(3)	-20,4682	67,0(3)	33,1	66,1	2,268(2)	4,679(3)
Cg11	Cg7	[2766]	5,029(3)	-11,1186	68,2(2)	1,9	70,1	1,712(2)	5,0260(19)
Cg11	Cg8	[2676]	5,316(3)	-20,6762	67,4(2)	20,6	64,7	2,276(2)	4,9770(19)
Cg12	Cg1	[2666]	5,050(3)	-4,3201	1,8(3)	47,6	45,9	3,517(3)	3,406(2)
Cg12	Cg2	[2666]	3,822(4)	-4,6736	2,9(3)	23,7	22,9	3,521(3)	3,498(3)
Cg12	Cg7	[2666]	4,309(3)	-4,4821	2,3(2)	36,7	35	3,529(3)	3,4543(19)
Cg12	Cg10	[1555]	5,479(3)	6,8166	69,8(3)	23,2	78,9	1,050(3)	5,037(2)
Cg12	Cg11	[1555]	4,918(4)	6,0772	69,0(3)	9,6	77,2	1,090(3)	4,849(2)
Cg12	Cg16	[1555]	5,060(3)	6,4443	69,4(2)	12,4	78,1	1,045(3)	4,9417(18)
Cg13	Cg1	[2666]	3,874(4)	-4,3201	1,6(3)	28,4	27,2	3,445(3)	3,407(2)
Cg13	Cg1	[2766]	5,991(4)	-11,0246	1,6(3)	57,5	57	3,259(3)	3,222(2)
Cg13	Cg2	[2666]	3,989(4)	-4,6736	2,6(3)	29	31,4	3,406(3)	3,490(3)
Cg13	Cg7	[2666]	3,739(3)	-4,4821	2,0(2)	22,6	23,2	3,437(3)	3,4505(19)
Cg13	Cg11	[1555]	5,225(4)	6,0772	68,7(3)	21,8	72,1	1,602(3)	4,852(2)
Cg13	Cg16	[1555]	5,869(3)	6,4443	69,1(2)	32,5	74,1	1,603(3)	4,9487(18)
Cg14	Cg3	[2676]	4,855(3)	-20,8761	2,3(3)	43,8	45,8	3,382(2)	3,504(3)
Cg14	Cg4	[2676]	3,797(4)	-20,4682	1,0(3)	25,1	25,7	3,421(2)	3,438(3)
Cg14	Cg8	[2676]	4,186(3)	-20,6762	1,6(2)	33,9	35,2	3,421(2)	3,474(2)
Cg14	Cg10	[1455]	4,811(3)	10,364	67,2(2)	17,1	76,5	1,123(2)	4,600(2)
Cg14	Cg16	[1455]	5,604(3)	9,975	67,1(2)	26,6	78,6	1,111(2)	5,0105(18)
Cg15	Cg3	[2676]	3,774(4)	-20,8761	3,4(3)	21,6	22,1	3,495(3)	3,508(3)
Cg15	Cg4	[2676]	4,120(4)	-20,4682	1,9(3)	34,3	32,4	3,477(3)	3,403(3)
Cg15	Cg8	[2676]	3,760(3)	-20,6762	2,6(2)	23,1	21,3	3,504(3)	3,459(2)
Cg15	Cg10	[1455]	4,766(3)	10,364	66,1(3)	15,7	73,6	1,348(2)	4,588(2)
Cg15	Cg11	[1455]	5,560(4)	9,5895	65,9(3)	14,8	75,9	1,359(2)	5,374(2)
Cg15	Cg16	[1455]	5,033(3)	9,975	66,0(2)	8,1	74,1	1,379(2)	4,9825(18)
Cg16	Cg1	[2766]	5,598(3)	-11,0246	69,3(2)	24,2	71,5	1,7740(18)	5,105(2)
Cg16	Cg2	[2766]	4,937(3)	-11,2381	67,8(2)	1,7	67,3	1,9047(18)	4,935(2)
Cg16	Cg3	[2676]	5,327(3)	-20,8761	67,7(2)	6,7	70,3	1,7949(18)	5,291(2)
Cg16	Cg4	[2676]	5,070(3)	-20,4682	67,1(2)	20,7	68,7	1,8406(18)	4,742(3)
Cg16	Cg7	[2766]	5,135(3)	-11,1186	68,58(17)	12,1	68,9	1,8485(18)	5,0206(19)
Cg16	Cg8	[2676]	5,054(3)	-20,6762	67,39(17)	7	68,7	1,8358(18)	5,0167(19)
Cg16	Cg12	[1655]	5,950(3)	13,7408	69,4(2)	39,7	73,3	1,7118(18)	4,576(3)
Cg17	Cg1	[2666]	4,332(3)	-4,3201	1,7(2)	38,1	36,5	3,481(2)	3,408(2)
Cg17	Cg2	[2666]	3,711(3)	-4,6736	2,8(2)	19,5	21	3,464(2)	3,497(3)
Cg17	Cg7	[2666]	3,845(3)	-4,4821	2,15(18)	26	25,1	3,483(2)	3,4550(19)
Cg17	Cg10	[1555]	5,983(3)	6,8166	69,6(2)	32,7	77	1,350(2)	5,037(2)
Cg17	Cg11	[1555]	4,923(3)	6,0772	68,9(2)	10,1	74,1	1,347(2)	4,847(2)
Cg17	Cg16	[1555]	5,341(3)	6,4443	69,25(17)	22,3	75,6	1,325(2)	4,9410(18)
Cg18	Cg3	[2676]	4,174(3)	-20,8761	2,8(2)	32,6	34,5	3,4407(19)	3,517(3)
Cg18	Cg4	[2676]	3,770(3)	-20,4682	1,4(3)	24,4	23,7	3,4511(19)	3,433(3)
Cg18	Cg8	[2676]	3,787(3)	-20,6762	2,03(18)	23,3	23,8	3,4644(19)	3,478(2)

Cg18	Cg10	[1455]	4,628(3)	10,364	66,7(2)	7,8	74,5	1,2351(18)	4,584(2)
Cg18	Cg11	[1455]	5,938(3)	9,5895	66,5(2)	24,9	78,3	1,2012(18)	5,387(2)
Cg18	Cg12	[1555]	5,984(3)	7,0877	15,4(2)	56,2	61,9	2,8216(19)	3,326(3)
Cg18	Cg16	[1455]	5,182(3)	9,975	66,61(17)	15,7	76,1	1,2443(18)	4,9870(18)

[1655]	1+X,Y,Z
[2666]	1-X,1-Y,1-Z
[2766]	2-X,1-Y,1-Z
[1555]	X,Y,Z
[2676]	1-X,2-Y,1-Z
[1455]	-1+X,Y,Z
[1576]	-X,2-Y,1-Z
[2766]	2-X,1-Y,1-Z
[2676]	1-X,2-Y,1-Z
[1655]	1+X,Y,Z
[2666]	1-X,1-Y,1-Z
[1555]	X,Y,Z
[1455]	-1+X,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
C11-H11	Cg16	[2766]	2,92	-2,77	18,59	139	3,694(6)	67
C22-H22	Cg10	[2676]	2,66	2,63	9,24	147	3,495(7)	64
C36-H36	Cg3	[1555]	2,67	-2,63	9,67	152	3,538(7)	64
C36-H36	Cg8	[1555]	2,75	-2,62	17,2	140	3,528(6)	63
C41-H41	Cg1	[1455]	2,74	2,63	16,44	131	3,444(6)	58
C41-H41	Cg7	[1455]	2,76	2,63	17,84	143	3,570(6)	57
C54-H54	Cg12	[1555]	2,69	2,67	6,46	154	3,567(7)	67
C54-H54	Cg17	[1555]	2,87	2,67	21,26	141	3,651(7)	67
C59-H59	Cg15	[1655]	2,62	-2,57	10,99	148	3,458(6)	60
C59-H59	Cg18	[1655]	2,7	-2,56	18,59	133	3,419(6)	60
C60-H60	Cg14	[1655]	2,91	-2,9	5,06	131	3,614(6)	46
C72-H72	Cg5	[2666]	2,69	-2,67	7,14	146	3,515(7)	62
C72-H72	Cg9	[2666]	2,99	-2,67	26,84	141	3,771(6)	63
C85-H85	Cg6	[2576]	2,8	2,75	10,04	143	3,603(7)	63

[2766]	2-X,1-Y,1-Z
[2676]	1-X,2-Y,1-Z
[1555]	X,Y,Z
[1455]	-1+X,Y,Z
[1555]	X,Y,Z
[1655]	1+X,Y,Z
[2666]	1-X,1-Y,1-Z
[2576]	-X,2-Y,1-Z

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

Cg(l)	x	y	z
Cg1	0,8430(3)	0,56290(14)	0,32998(8)
Cg2	0,8320(3)	0,54548(16)	0,24711(8)
Cg3	0,5367(3)	0,93185(16)	0,26387(8)
Cg4	0,5100(3)	0,96707(16)	0,18230(8)
Cg5	0,1458(2)	0,74838(13)	0,30889(8)
Cg6	0,2012(3)	0,76205(15)	0,22607(8)
Cg7	0,8376(2)	0,55430(12)	0,28852(6)
Cg8	0,5231(2)	0,94937(12)	0,22309(6)
Cg9	0,1736(2)	0,75524(11)	0,26753(6)
Cg10	0,8615(2)	0,76078(12)	0,79185(8)
Cg11	0,8075(3)	0,74495(15)	0,71215(8)
Cg12	0,4726(3)	0,56840(16)	0,76457(8)
Cg13	0,4933(3)	0,52913(16)	0,68308(8)
Cg14	0,1671(3)	0,93473(14)	0,84193(7)
Cg15	0,1626(3)	0,95385(16)	0,75840(8)
Cg16	0,8348(2)	0,75263(11)	0,75200(6)
Cg17	0,4831(2)	0,54874(13)	0,72383(6)
Cg18	0,1646(2)	0,94423(12)	0,80017(6)

Nr	Donor	--- H....	Acceptor [ARU]	D - H	H...A	D...A	D - H...A
1	O7	--H7	..O8 [2676.01]	0.81	2.05	2.819(4)	158
2	O8	--H8A	..O3 [2676.01]	0.92	1.90	2.754(5)	154
3	O15	--H15	..O16 [2667.02]	0.77	2.11	2.817(4)	153
4	O16	--H16	..O11 [2667.02]	0.84	2.00	2.800(5)	159

Translation of ARU-Code to CIF and Equivalent Position Code

[2676.] = [2_676] = 1-x,2-y,1-z
 [1655.] = [1_655] = 1+x,y,z
 [2667.] = [2_667] = 1-x,1-y,2-z
 [1455.] = [1_455] = -1+x,y,z

Table S3. Non-coordinative interactions in **2**.

6-Membered Ring (1)	N1	-->	C43	-->	C44	-->	C45	-->	C46	-->	C47	-->
6-Membered Ring (2)	N2	-->	C51	-->	C50	-->	C52	-->	C53	-->	C54	-->
6-Membered Ring (3)	C5	-->	C6	-->	C7	-->	C12	-->	C13	-->	C14	-->
6-Membered Ring (4)	C7	-->	C8	-->	C9	-->	C10	-->	C11	-->	C12	-->
6-Membered Ring (5)	C19	-->	C20	-->	C21	-->	C26	-->	C27	-->	C28	-->
6-Membered Ring (6)	C21	-->	C22	-->	C23	-->	C24	-->	C25	-->	C26	-->
6-Membered Ring (7)	C33	-->	C34	-->	C35	-->	C40	-->	C41	-->	C42	-->
6-Membered Ring (8)	C35	-->	C36	-->	C37	-->	C38	-->	C39	-->	C40	-->
6-Membered Ring (9)	C43	-->	C44	-->	C48	-->	C49	-->	C50	-->	C51	-->
6-Membered Ring (10)	C33A	-->	C34A	-->	C35A	-->	C40A	-->	C41A	-->	C42A	-->
6-Membered Ring (11)	C35A	-->	C36A	-->	C37A	-->	C38A	-->	C39A	-->	C40A	-->

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.)
- Slippage = Distance between Cg(I) and Perpendicular Projection 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	[3666]	3,556(2)	-12,5275	0,00(17)	20,4	20,4	3,3329(14)	3,3331(14)
Cg1	Cg2	[3666]	5,543(2)	-12,7798	6,01(17)	50,4	56,1	3,0898(14)	3,5313(14)
Cg1	Cg8	[2556]	4,750(3)	15,3989	36,1(2)	28,3	55,1	2,7181(14)	4,184(2)
Cg1	Cg9	[3666]	3,922(2)	-12,5885	2,06(17)	31	32,8	3,2975(14)	3,3607(15)
Cg1	Cg11	[2556]	4,585(9)	16,3707	31,9(8)	34,4	47,4	3,1048(14)	3,784(8)
Cg2	Cg1	[3666]	5,543(2)	-12,5275	6,01(17)	56,1	50,4	3,5313(14)	3,0899(14)
Cg2	Cg4	[4454]	5,183(2)	-2,3495	83,34(16)	30,1	53,7	3,0716(14)	4,4834(14)
Cg2	Cg7	[2556]	4,218(2)	15,4047	32,2(2)	14,5	43,7	3,0480(14)	4,083(2)
Cg2	Cg8	[2556]	4,507(3)	15,3989	31,8(2)	24,8	46,8	3,0827(14)	4,090(2)
Cg2	Cg10	[2556]	4,836(7)	15,3594	32,6(7)	19,3	51,3	3,0251(14)	4,563(8)
Cg2	Cg11	[2556]	3,910(8)	16,3707	28,1(8)	18,5	34,1	3,2367(14)	3,706(8)
Cg3	Cg5	[1555]	5,906(2)	6,4425	20,70(17)	53	46,4	4,0750(15)	3,5558(14)
Cg3	Cg7	[2546]	3,558(3)	5,2891	5,6(2)	7,6	4,6	3,5468(14)	3,527(2)
Cg3	Cg8	[2546]	4,386(3)	5,4665	3,7(2)	40,5	36,8	3,5100(14)	3,334(2)
Cg3	Cg10	[2546]	3,629(9)	5,1798	6,1(7)	16	11,2	3,5594(14)	3,489(8)
Cg3	Cg11	[2546]	4,183(9)	6,5622	7,6(8)	38,6	31	3,5846(14)	3,270(9)
Cg4	Cg1	[2646]	5,8315(19)	-21,2245	83,48(17)	44	80,5	0,9652(14)	4,1928(14)
Cg4	Cg2	[4555]	5,183(2)	24,1422	83,34(16)	53,7	30,1	4,4834(14)	3,0717(14)
Cg4	Cg7	[2546]	4,299(2)	5,2891	5,9(2)	34,1	38,1	3,3832(15)	3,561(2)
Cg4	Cg8	[2546]	4,483(3)	5,4665	4,1(2)	41,2	40,8	3,3957(15)	3,376(2)
Cg4	Cg9	[4555]	5,732(2)	24,5118	83,31(17)	54,2	39,6	4,4184(14)	3,3512(15)
Cg4	Cg10	[2546]	3,792(8)	5,1798	6,5(7)	22,7	27,1	3,3754(15)	3,499(8)
Cg4	Cg11	[2546]	4,832(8)	6,5622	6,8(8)	46,3	42,5	3,5638(15)	3,336(9)

Cg5	Cg2	[2546]	5,102(2)	-15,2659	74,70(17)	20	85,8	0,3750(14)	4,7938(14)
Cg5	Cg3	[1555]	5,906(2)	9,0743	20,70(17)	46,4	53	3,5559(14)	4,0750(15)
Cg5	Cg4	[3657]	5,766(2)	-11,5107	22,27(17)	52,3	73,7	1,6149(14)	3,5296(15)
Cg5	Cg7	[2556]	4,939(3)	15,4047	19,3(2)	39,4	58,6	2,5713(15)	3,818(2)
Cg5	Cg8	[2556]	5,439(3)	15,3989	19,8(2)	45,7	61,8	2,5689(15)	3,802(2)
Cg5	Cg10	[2556]	4,197(9)	15,3594	19,0(7)	33	52,1	2,5806(15)	3,518(9)
Cg6	Cg2	[2546]	4,857(2)	-15,2659	73,92(17)	10,5	79,8	0,8631(16)	4,7757(14)
Cg6	Cg4	[3657]	5,775(2)	-11,5107	22,82(17)	51,9	74,5	1,5393(15)	3,5632(15)
Cg6	Cg7	[2556]	5,716(3)	15,4047	19,4(2)	48,6	64,7	2,4403(15)	3,781(2)
Cg6	Cg9	[2546]	5,385(2)	-16,1932	73,87(17)	19,1	80,4	0,9008(16)	5,0888(15)
Cg6	Cg10	[2556]	5,162(8)	15,3594	19,1(7)	47,8	61,9	2,4309(15)	3,469(9)
Cg7	Cg2	[2546]	4,218(2)	-15,2659	32,2(2)	43,7	14,5	4,083(2)	3,0480(14)
Cg7	Cg3	[2556]	3,558(3)	0,913	5,6(2)	4,6	7,6	3,526(2)	3,5469(14)
Cg7	Cg4	[2556]	4,299(2)	0,456	5,9(2)	38,1	34,1	3,560(2)	3,3833(15)
Cg7	Cg5	[2546]	4,939(3)	-0,8887	19,3(2)	58,6	39,4	3,818(2)	2,5713(15)
Cg8	Cg1	[2546]	4,751(3)	-16,6945	36,1(2)	55,1	28,3	4,184(2)	2,7180(14)
Cg8	Cg2	[2546]	4,507(3)	-15,2659	31,8(2)	46,8	24,8	4,090(2)	3,0827(14)
Cg8	Cg3	[2556]	4,386(3)	0,913	3,7(2)	36,8	40,5	3,334(2)	3,5100(14)
Cg8	Cg4	[2556]	4,483(3)	0,456	4,1(2)	40,8	41,2	3,376(2)	3,3958(15)
Cg9	Cg1	[3666]	3,922(2)	-12,5275	2,06(17)	32,8	31	3,3608(15)	3,2976(14)
Cg9	Cg4	[4454]	5,732(2)	-2,3495	83,31(17)	39,6	54,2	3,3511(15)	4,4183(14)
Cg9	Cg7	[2556]	5,284(2)	15,4047	34,9(2)	36,8	64,5	2,2718(15)	4,230(2)
Cg9	Cg8	[2556]	4,573(3)	15,3989	34,6(2)	25,9	60,5	2,2532(15)	4,114(2)
Cg9	Cg9	[3666]	5,448(2)	-12,5885	0,00(17)	52,9	52,9	3,2871(15)	3,2870(15)
Cg9	Cg10	[2556]	5,861(7)	15,3594	35,2(7)	36,2	67,3	2,2601(15)	4,729(8)
Cg9	Cg11	[2556]	3,940(8)	16,3707	30,6(8)	19,4	48,9	2,5890(15)	3,717(8)
Cg10	Cg2	[2546]	4,836(7)	-15,2659	32,6(7)	51,3	19,3	4,563(8)	3,0251(14)
Cg10	Cg3	[2556]	3,630(9)	0,913	6,1(7)	11,2	16	3,490(8)	3,5595(14)
Cg10	Cg4	[2556]	3,792(8)	0,456	6,5(7)	27,1	22,7	3,499(8)	3,3754(15)
Cg10	Cg5	[2546]	4,196(9)	-0,8887	19,0(7)	52,1	33	3,517(9)	2,5806(15)
Cg11	Cg1	[2546]	4,585(9)	-16,6945	31,9(8)	47,4	34,4	3,784(8)	3,1047(14)
Cg11	Cg2	[2546]	3,910(8)	-15,2659	28,1(8)	34,1	18,5	3,707(8)	3,2367(14)
Cg11	Cg3	[2556]	4,183(9)	0,913	7,6(8)	31	38,6	3,270(9)	3,5847(14)
Cg11	Cg4	[2556]	4,831(8)	0,456	6,8(8)	42,5	46,3	3,336(9)	3,5638(15)
Cg11	Cg9	[2546]	3,940(8)	-16,1932	30,6(8)	48,9	19,4	3,718(8)	2,5891(15)

[3666]	1-X,1-Y,1-Z
[2556]	1/2-X,1/2+Y,3/2-Z
[4454]	-1/2+X,1/2-Y,-1/2+Z
[1555]	X,Y,Z
[2546]	1/2-X,-1/2+Y,3/2-Z
[2646]	3/2-X,-1/2+Y,3/2-Z
[4555]	1/2+X,1/2-Y,1/2+Z
[3657]	1-X,-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
C39-H39	Cg9	[2546]	2,81	2,81	1,16	124	3,427(5)	33
C52-H52	Cg6	[2556]	2,6	-2,55	10,98	159	3,505(4)	72
C37A-H37A	Cg9	[2546]	2,68	2,55	17,88	102	3,03(2)	29
C42A-H42A	Cg5	[2546]	2,88	2,86	6,14	105	3,255(17)	15

[2546]	1/2-X,-1/2+Y,3/2-Z
[2556]	1/2-X,1/2+Y,3/2-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
C29-F8	Cg4	[4454]	3,205(3)	3,197	4,09	139,1(2)	4,309(4)	47,45

[4454]	-1/2+X,1/2-Y,-1/2+Z
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The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,54807(8)	0,51863(12)	0,57333(6)
Cg2	0,31908(8)	0,61868(12)	0,61067(6)
Cg3	0,52212(8)	-0,01030(12)	0,84136(6)
Cg4	0,60243(8)	-0,12723(12)	0,91667(6)
Cg5	0,39938(8)	0,42783(12)	0,89698(6)
Cg6	0,27842(10)	0,49468(12)	0,93401(7)
Cg7	0,08508(13)	0,25178(17)	0,72568(8)
Cg8	-0,04602(13)	0,17590(18)	0,74540(9)
Cg9	0,43470(10)	0,65193(12)	0,56290(6)
Cg10	0,0560(5)	0,2113(7)	0,6932(3)
Cg11	-0,0116(5)	0,2294(8)	0,7747(3)

Table S4. Non-coordinative interactions in **2a**.

6-Membered Ring (1)	N1	-->	C43	-->	C44	-->	C45	-->	C46	-->	C47	-->
6-Membered Ring (2)	N2	-->	C48	-->	C49	-->	C50	-->	C51	-->	C52	-->
6-Membered Ring (3)	C5	-->	C6	-->	C7	-->	C12	-->	C13	-->	C14	-->
6-Membered Ring (4)	C7	-->	C8	-->	C9	-->	C10	-->	C11	-->	C12	-->
6-Membered Ring (5)	C19	-->	C20	-->	C21	-->	C26	-->	C27	-->	C28	-->
6-Membered Ring (6)	C21	-->	C22	-->	C23	-->	C24	-->	C25	-->	C26	-->
6-Membered Ring (7)	C33	-->	C34	-->	C35	-->	C40	-->	C41	-->	C42	-->
6-Membered Ring (8)	C35	-->	C36	-->	C37	-->	C38	-->	C39	-->	C40	-->
6-Membered Ring (9)	C46	-->	C47	-->	C48	-->	C49	-->	C54	-->	C53	-->

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.)
- Slippage = Distance between Cg(I) and Perpendicular Projection 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	[2767]	5,4804(19)	-4,29	7,00(15)	57,8	50,8	3,4601(13)	2,9220(13)
Cg1	Cg5	[1655]	4,553(2)	26,3104	52,85(16)	43,9	11,6	4,4597(14)	3,2807(13)
Cg1	Cg6	[1655]	5,473(2)	26,6446	52,26(18)	45,5	34,4	4,5149(14)	3,8346(15)
Cg1	Cg6	[2677]	4,915(2)	-23,5413	52,26(18)	26	73,3	1,4116(14)	4,4170(15)
Cg2	Cg1	[2767]	5,4804(19)	-6,1	7,00(15)	50,8	57,8	2,9220(13)	3,4601(13)
Cg2	Cg2	[2767]	3,4426(18)	-4,29	0,00(15)	20,1	20,1	3,2333(13)	3,2334(13)
Cg2	Cg5	[2677]	4,7660(18)	-23,143	51,65(16)	11,7	48,7	3,1427(14)	4,6662(13)
Cg2	Cg6	[2677]	4,6863(19)	-23,5413	51,31(17)	19,9	47,7	3,1543(14)	4,4057(15)
Cg2	Cg9	[2767]	3,8415(18)	-4,9186	2,38(15)	31,8	33,9	3,1902(13)	3,2658(13)
Cg3	Cg3	[2766]	3,9872(18)	-12,4365	0,00(15)	34,4	34,4	3,2894(13)	3,2894(13)
Cg3	Cg4	[2766]	4,973(2)	-12,2194	1,22(16)	48,7	49,1	3,2550(13)	3,2830(15)
Cg3	Cg7	[1555]	5,4100(19)	4,8695	59,91(16)	21,5	39,3	4,1850(13)	5,0340(14)
Cg3	Cg7	[1655]	4,7061(19)	-0,8739	59,91(16)	11,8	70,7	1,5584(13)	4,6073(14)
Cg3	Cg8	[1555]	5,510(2)	4,5937	59,87(17)	30,5	40,1	4,2158(13)	4,7496(17)
Cg3	Cg8	[1655]	5,379(2)	-1,1496	59,87(17)	24,6	73,5	1,5276(13)	4,8917(17)
Cg4	Cg3	[2766]	4,973(2)	-12,4365	1,22(16)	49,1	48,7	3,2830(15)	3,2550(13)
Cg4	Cg7	[1555]	5,919(2)	4,8695	58,86(17)	30,9	52,2	3,6278(15)	5,0809(14)
Cg4	Cg7	[1655]	5,383(2)	-0,8739	58,86(17)	31,7	66,9	2,1156(15)	4,5783(14)
Cg4	Cg8	[1555]	4,957(2)	4,5937	58,85(18)	15,7	44,3	3,5504(15)	4,7720(17)
Cg4	Cg8	[1655]	4,921(2)	-1,1496	58,85(18)	6,7	63,5	2,1929(15)	4,8873(17)
Cg5	Cg1	[1455]	4,553(2)	10,3432	52,85(16)	11,6	43,9	3,2806(13)	4,4596(14)
Cg5	Cg2	[2677]	4,7660(18)	-16,8019	51,65(16)	48,7	11,7	4,6662(13)	3,1427(14)
Cg5	Cg5	[2677]	4,497(2)	-23,143	0,00(17)	40,4	40,4	3,4264(15)	3,4264(15)
Cg5	Cg6	[2577]	4,989(2)	-17,0639	1,66(18)	51,1	52	3,0687(15)	3,1315(17)

Cg5	Cg6	[2677]	4,735(2)	-23,5413	1,66(18)	43	43,9	3,4087(15)	3,4624(17)
Cg5	Cg9	[1455]	4,994(2)	9,328	51,81(16)	22,5	47,3	3,3852(13)	4,6151(15)
Cg6	Cg1	[1455]	5,473(2)	10,3432	52,26(18)	34,4	45,5	3,8346(15)	4,5148(14)
Cg6	Cg2	[2677]	4,6863(19)	-16,8019	51,31(17)	47,7	19,9	4,4057(15)	3,1543(14)
Cg6	Cg5	[2577]	4,989(2)	-16,5491	1,66(18)	52	51,1	3,1316(17)	3,0688(15)
Cg6	Cg5	[2677]	4,735(2)	-23,143	1,66(18)	43,9	43	3,4623(17)	3,4086(15)
Cg6	Cg6	[2577]	4,623(3)	-17,0639	0,00(19)	47,8	47,8	3,1034(17)	3,1034(17)
Cg6	Cg9	[1455]	4,763(2)	9,328	51,39(17)	14,9	38,1	3,7461(15)	4,6031(15)
Cg7	Cg3	[1555]	5,4100(19)	15,7258	59,91(16)	39,3	21,5	5,0339(14)	4,1850(13)
Cg7	Cg3	[2766]	4,5491(19)	-12,4365	59,91(16)	9,6	67,5	1,7446(14)	4,4851(13)
Cg7	Cg4	[1555]	5,919(2)	15,4819	58,86(17)	52,2	30,9	5,0809(14)	3,6278(15)
Cg7	Cg4	[2766]	5,452(2)	-12,2194	58,86(17)	22,4	70,5	1,8184(14)	5,0423(15)
Cg8	Cg3	[1555]	5,510(2)	15,7258	59,87(17)	40,1	30,5	4,7496(17)	4,2157(13)
Cg8	Cg3	[2766]	4,911(2)	-12,4365	59,87(17)	23,3	72,7	1,4602(17)	4,5106(13)
Cg8	Cg4	[1555]	4,957(2)	15,4819	58,85(18)	44,3	15,7	4,7720(17)	3,5504(15)
Cg8	Cg8	[2676]	5,274(2)	-8,0317	0,00(18)	49,3	49,3	3,4379(16)	3,4380(16)
Cg9	Cg2	[2767]	3,8416(18)	-4,29	2,38(15)	33,9	31,8	3,2658(13)	3,1903(13)
Cg9	Cg5	[1655]	4,994(2)	26,3104	51,81(16)	47,3	22,5	4,6151(15)	3,3853(13)
Cg9	Cg5	[2677]	5,380(2)	-23,143	51,81(16)	28,7	74,4	1,4476(15)	4,7183(13)
Cg9	Cg6	[1655]	4,763(2)	26,6446	51,39(17)	38,1	14,9	4,6031(15)	3,7461(15)
Cg9	Cg6	[2677]	4,661(2)	-23,5413	51,39(17)	20,8	71,2	1,4997(15)	4,3574(15)
Cg9	Cg9	[2767]	5,413(2)	-4,9186	0,00(14)	54,1	54,1	3,1715(13)	3,1715(13)

[2767]	2-X,1-Y,2-Z
[1655]	1+X,Y,Z
[2677]	1-X,2-Y,2-Z
[2766]	2-X,1-Y,1-Z
[1555]	X,Y,Z
[1455]	-1+X,Y,Z
[2577]	-X,2-Y,2-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
C13-H13	Cg7	[2766]	2,58	-2,52	12,3	135	3,326(4)	57
C14-H14	Cg8	[2766]	2,99	-2,98	3,16	134	3,706(3)	41
C25-H25	Cg9	[2677]	2,57	2,56	4,51	143	3,377(4)	50

C41-H41	Cg3	[1455]	2,6	2,58	7,18	144	3,421(4)	60
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[2766]	2-X,1-Y,1-Z
[2677]	1-X,2-Y,2-Z
[1455]	-1+X,Y,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
C29-F8	Cg1	[1455]	3,344(17)	-3,322	6,47	117,5(13)	4,12(2)	20,99

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

Cg(I)	x	y	z
Cg1	1,21165(15)	0,69882(11)	0,85781(7)
Cg2	0,89038(15)	0,63252(10)	0,98796(6)
Cg3	1,11037(12)	0,59455(11)	0,53152(6)
Cg4	1,07437(15)	0,73625(12)	0,44987(6)
Cg5	0,32493(16)	0,98707(11)	0,94373(6)
Cg6	0,20030(18)	0,98532(12)	1,05123(7)
Cg7	0,52608(14)	0,67630(12)	0,58244(6)
Cg8	0,54367(16)	0,78335(13)	0,48605(7)
Cg9	1,12713(17)	0,66110(10)	0,96519(7)

Table S5: Non-coordinative interactions in 3.

6-Membered Ring (1)	N1	-->	C43	-->	C44	-->	C45	-->	C46	-->	C47	-->								
6-Membered Ring (2)	N2	-->	C48	-->	C49	-->	C50	-->	C51	-->	C52	-->								
6-Membered Ring (3)	C5	-->	C6	-->	C7	-->	C12	-->	C13	-->	C14	-->								
6-Membered Ring (4)	C7	-->	C8	-->	C9	-->	C10	-->	C11	-->	C12	-->								
6-Membered Ring (5)	C19	-->	C20	-->	C21	-->	C26	-->	C27	-->	C28	-->								
6-Membered Ring (6)	C21	-->	C22	-->	C23	-->	C24	-->	C25	-->	C26	-->								
6-Membered Ring (7)	C33	-->	C34	-->	C35	-->	C40	-->	C41	-->	C42	-->								
6-Membered Ring (8)	C35	-->	C36	-->	C37	-->	C38	-->	C39	-->	C40	-->								
10-Membered Ring (9)	C5	-->	C6	-->	C7	-->	C8	-->	C9	-->	C10	-->	C11	-->	C12	-->	C13	-->	C14	-->
10-Membered Ring (10)	C19	-->	C20	-->	C21	-->	C22	-->	C23	-->	C24	-->	C25	-->	C26	-->	C27	-->	C28	-->
10-Membered Ring (11)	C33	-->	C34	-->	C35	-->	C36	-->	C37	-->	C38	-->	C39	-->	C40	-->	C41	-->	C42	-->

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.)
- Slippage = Distance between Cg(I) and Perpendicular Projection 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	[3565]	5,0674(14)	-11,2894	0,02(12)	47,9	47,9	3,3958(10)	3,3958(10)
Cg1	Cg2	[3565]	3,8380(14)	-10,8471	7,23(12)	25,5	20,6	3,5933(10)	3,4653(10)
Cg1	Cg6	[4554]	5,8745(15)	-1,6068	37,93(12)	44,2	58,3	3,0905(10)	4,2145(10)
Cg1	Cg10	[4554]	5,8364(13)	-1,5165	39,50(10)	35,2	58,6	3,0375(10)	4,7676(7)
Cg2	Cg1	[3565]	3,8380(14)	-11,2894	7,23(12)	20,6	25,5	3,4653(10)	3,5933(10)
Cg2	Cg5	[4554]	5,8450(13)	-1,4924	34,31(11)	30,3	61,9	2,7508(9)	5,0486(9)
Cg2	Cg6	[4554]	4,1728(14)	-1,6068	31,02(11)	13,3	44,3	2,9852(10)	4,0605(10)
Cg2	Cg10	[4554]	4,9325(12)	-1,5165	32,61(9)	22,4	53,9	2,9080(10)	4,5594(7)
Cg3	Cg2	[2555]	5,9588(13)	15,724	67,46(11)	53,7	66,1	2,4115(9)	3,5305(9)
Cg3	Cg2	[3565]	5,2500(13)	-10,8471	79,34(11)	28,9	73	1,5308(9)	4,5952(9)
Cg3	Cg5	[2555]	4,5181(13)	10,7451	45,31(10)	44,2	17,2	4,3151(9)	3,2410(9)
Cg3	Cg6	[2555]	4,7906(13)	11,3291	48,50(10)	23,2	27,3	4,2579(9)	4,4022(9)
Cg3	Cg8	[3666]	5,2896(13)	-12,0114	68,18(10)	26,5	88,4	0,1471(8)	4,7346(9)
Cg3	Cg10	[2555]	4,4982(11)	11,0848	46,96(8)	31,8	16,1	4,3222(9)	3,8250(7)
Cg4	Cg2	[3565]	5,6459(14)	-10,8471	79,33(11)	35,4	69,6	1,9679(9)	4,6021(9)
Cg4	Cg5	[2555]	5,3568(13)	10,7451	45,39(10)	52,3	44,3	3,8367(9)	3,2761(9)
Cg4	Cg6	[2555]	4,8741(13)	11,3291	48,56(11)	25,2	38,9	3,7939(9)	4,4101(9)
Cg4	Cg10	[2555]	4,9773(12)	11,0848	47,03(9)	39,4	39,3	3,8515(9)	3,8465(7)
Cg5	Cg3	[2545]	4,5181(13)	-3,5089	45,31(10)	17,2	44,2	3,2410(9)	4,3151(9)
Cg5	Cg4	[2545]	5,3568(13)	-3,391	45,39(10)	44,3	52,3	3,2761(9)	3,8367(9)
Cg5	Cg4	[2645]	5,9875(13)	-8,5848	45,39(10)	53,1	71,3	1,9177(9)	3,5909(9)
Cg5	Cg7	[1555]	5,3740(13)	8,4857	73,30(10)	21,2	75,6	1,3340(9)	5,0112(9)
Cg5	Cg8	[1555]	4,8724(13)	8,9142	71,24(10)	6	72,3	1,4799(9)	4,8454(9)

Cg5	Cg9	[2545]	4,8014(12)	-3,4625	45,36(9)	31,9	47,4	3,2468(9)	4,0756(7)
Cg5	Cg11	[1555]	4,9794(12)	8,6726	72,31(9)	8,4	73,9	1,3818(9)	4,9261(7)
Cg6	Cg1	[4555]	5,8745(15)	-0,2313	37,93(12)	58,3	44,2	4,2146(10)	3,0905(10)
Cg6	Cg2	[4555]	4,1728(14)	-1,0871	31,02(11)	44,3	13,3	4,0605(10)	2,9852(10)
Cg6	Cg3	[2545]	4,7906(13)	-3,5089	48,50(10)	27,3	23,2	4,4022(9)	4,2579(9)
Cg6	Cg4	[2545]	4,8740(13)	-3,391	48,56(11)	38,9	25,2	4,4101(9)	3,7939(9)
Cg6	Cg8	[1555]	5,2699(13)	8,9142	72,12(11)	22,6	87	0,2715(10)	4,8653(9)
Cg6	Cg9	[2545]	4,6741(12)	-3,4625	48,54(9)	30,5	19,9	4,3953(9)	4,0257(7)
Cg6	Cg11	[1555]	5,7411(12)	8,6726	73,13(9)	29,1	86,5	0,3507(10)	5,0150(7)
Cg7	Cg4	[2645]	4,7850(13)	-8,5848	81,72(10)	8,4	87,2	0,2332(8)	4,7340(9)
Cg7	Cg7	[3666]	3,6842(13)	-11,7406	0,00(10)	27,9	27,9	3,2548(9)	3,2548(9)
Cg7	Cg8	[3666]	5,2516(13)	-12,0114	2,85(10)	51,2	53,3	3,1360(9)	3,2934(9)
Cg7	Cg11	[3666]	4,3700(12)	-11,8957	1,39(8)	41,4	42,5	3,2197(9)	3,2774(7)
Cg8	Cg4	[2645]	5,0108(13)	-8,5848	78,87(10)	18,7	68,4	1,8475(9)	4,7456(9)
Cg8	Cg7	[3666]	5,2515(13)	-11,7406	2,85(10)	53,3	51,2	3,2934(9)	3,1359(9)
Cg9	Cg2	[2555]	5,9953(12)	15,724	67,06(9)	53,9	77,5	1,2977(7)	3,5295(9)
Cg9	Cg2	[3565]	5,3107(12)	-10,8471	79,35(9)	30,2	70,8	1,7486(7)	4,5886(9)
Cg9	Cg5	[2555]	4,8013(12)	10,7451	45,36(9)	47,4	31,9	4,0756(7)	3,2468(9)
Cg9	Cg6	[2555]	4,6740(12)	11,3291	48,54(9)	19,9	30,5	4,0257(7)	4,3952(9)
Cg9	Cg8	[3666]	5,6557(12)	-12,0114	68,28(9)	33,2	89,5	0,0510(7)	4,7311(9)
Cg9	Cg10	[2555]	4,5825(10)	11,0848	47,00(6)	33,4	26,9	4,0866(7)	3,8244(7)
Cg10	Cg1	[4555]	5,8364(13)	-0,2313	39,50(10)	58,6	35,2	4,7675(7)	3,0375(10)
Cg10	Cg2	[4555]	4,9325(12)	-1,0871	32,61(9)	53,9	22,4	4,5594(7)	2,9080(10)
Cg10	Cg3	[2545]	4,4981(11)	-3,5089	46,96(8)	16,1	31,8	3,8249(7)	4,3222(9)
Cg10	Cg4	[2545]	4,9772(12)	-3,391	47,03(9)	39,3	39,4	3,8464(7)	3,8515(9)
Cg10	Cg7	[1555]	5,7851(12)	8,4857	73,70(9)	29	85,3	0,4765(7)	5,0600(9)
Cg10	Cg8	[1555]	4,9203(12)	8,9142	71,70(9)	11,4	83	0,6026(7)	4,8230(9)
Cg10	Cg9	[2545]	4,5825(10)	-3,4625	47,00(6)	26,9	33,4	3,8244(7)	4,0867(7)
Cg10	Cg11	[1555]	5,2276(10)	8,6726	72,73(6)	19,1	84,4	0,5141(7)	4,9394(7)
Cg11	Cg4	[2645]	4,7407(12)	-8,5848	80,32(9)	5,5	77,3	1,0386(7)	4,7186(9)
Cg11	Cg7	[3666]	4,3700(12)	-11,7406	1,39(8)	42,5	41,4	3,2774(7)	3,2197(9)
Cg11	Cg9	[2645]	5,9339(10)	-8,5931	79,88(6)	3,5	79,6	1,0734(7)	5,9228(7)
Cg11	Cg11	[3666]	5,2546(10)	-11,8957	0,00(6)	52,2	52,2	3,2231(7)	3,2231(7)

[3565]	-X,1-Y,-Z
[4554]	X,1/2-Y,-1/2+Z
[2555]	-X,1/2+Y,1/2-Z
[3666]	1-X,1-Y,1-Z
[2545]	-X,-1/2+Y,1/2-Z
[2645]	1-X,-1/2+Y,1/2-Z
[1555]	X,Y,Z

[4555]	X,1/2-Y,1/2+Z
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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	Cg11	[2655]	2,86	-2,7	19,39	132	3,566(2)	60
C10-H10	Cg7	[2655]	2,84	-2,75	14,23	135	3,578(2)	58
C36-H36	Cg5	[1555]	2,75	2,64	16,34	146	3,575(2)	70
C36-H36	Cg10	[1555]	2,65	2,62	9,49	159	3,558(2)	70

[2655]	1-X,1/2+Y,1/2-Z
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[1555]	X,Y,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
C15-F4	Cg4	[2645]	3,2210(16)	3,208	5,17	132,94(12)	4,252(2)	41,72
C15-F4	Cg9	[2645]	3,4319(15)	3,21	20,7	150,86(12)	4,652(2)	41,39

[2645]	1-X,-1/2+Y,1/2-Z
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The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,22101(9)	0,48531(4)	-0,01282(5)
Cg2	-0,02996(8)	0,38490(4)	0,08647(5)
Cg3	0,10240(8)	0,70712(4)	0,18341(5)
Cg4	0,21968(8)	0,78052(4)	0,12683(5)
Cg5	0,26169(8)	0,26870(4)	0,42407(5)
Cg6	0,15983(8)	0,26193(5)	0,53719(5)
Cg7	0,59099(8)	0,43501(4)	0,49053(5)
Cg8	0,58517(8)	0,36154(4)	0,58790(5)
Cg9	0,16100(6)	0,74377(3)	0,15505(4)
Cg10	0,21113(6)	0,26545(3)	0,48076(4)
Cg11	0,58811(6)	0,39818(3)	0,53906(4)

Table S6. Non-coordinative interactions in **4**.

6-Membered Ring (1) N1 --> C43 --> C44 --> C45 --> C46 --> C47 -->
 6-Membered Ring (2) N2 --> C49 --> C50 --> C51 --> C52 --> C53 -->
 6-Membered Ring (3) C5 --> C6 --> C7 --> C12 --> C13 --> C14 -->
 6-Membered Ring (4) C7 --> C8 --> C9 --> C10 --> C11 --> C12 -->
 6-Membered Ring (5) C19 --> C20 --> C21 --> C26 --> C27 --> C28 -->
 6-Membered Ring (6) C21 --> C22 --> C23 --> C24 --> C25 --> C26 -->
 6-Membered Ring (7) C33 --> C34 --> C35 --> C40 --> C41 --> C42 -->
 6-Membered Ring (8) C35 --> C36 --> C37 --> C38 --> C39 --> C40 -->

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.)
- Slippage = Distance between Cg(I) and Perpendicular Projection of Cg(J) on Ring I (Ang.).

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg	Alpha	Beta	Gamma	CgI_Perp	CgJ_Perp	Slippage
Cg1	Cg7	[4465]	4,998(2)	-1,2785	42,94(17)	28	63,3	2,2450(16)	4,4112(14)
Cg1	Cg8	[3654]	5,894(2)	8,5233	85,22(18)	25,1	79,6	1,0596(16)	5,3386(15)
Cg2	Cg3	[1565]	5,547(2)	13,43	29,49(18)	58,9	34,9	4,5484(15)	2,8654(15)
Cg2	Cg6	[1565]	4,688(2)	-2,859	40,52(18)	58,3	28,7	4,1111(15)	2,4628(16)
Cg2	Cg7	[4465]	4,669(2)	-1,2785	55,79(17)	21,3	41,2	3,5130(14)	4,3500(14)
Cg2	Cg8	[4465]	4,893(2)	-0,3895	55,89(18)	20	44,2	3,5063(14)	4,5989(15)
Cg3	Cg2	[1545]	5,547(2)	2,9256	29,49(18)	34,9	58,9	2,8656(15)	4,5484(15)
Cg3	Cg5	[4555]	3,588(2)	11,7409	4,86(17)	16,5	16	3,4485(15)	3,4397(15)
Cg3	Cg6	[4555]	3,856(2)	11,7256	5,71(18)	23,1	26,9	3,4388(15)	3,5458(15)
Cg4	Cg5	[4555]	3,829(2)	11,7409	8,26(18)	25,4	33,4	3,1950(16)	3,4574(15)
Cg4	Cg6	[4555]	5,242(2)	11,7256	8,74(18)	44,5	52,7	3,1765(16)	3,7372(15)
Cg5	Cg2	[1545]	4,386(2)	2,9256	39,38(17)	21,3	60,2	2,1814(15)	4,0866(15)
Cg5	Cg3	[4455]	3,588(2)	-0,5887	4,86(17)	16	16,5	3,4399(15)	3,4487(15)
Cg5	Cg4	[4455]	3,829(2)	-1,4134	8,26(18)	33,4	25,4	3,4575(15)	3,1950(16)
Cg6	Cg1	[1545]	5,433(2)	0,9641	55,69(18)	31,9	76	1,3145(15)	4,6106(15)
Cg6	Cg2	[1545]	4,688(2)	2,9256	40,52(18)	28,7	58,3	2,4627(16)	4,1111(15)
Cg6	Cg3	[4455]	3,856(2)	-0,5887	5,71(18)	26,9	23,1	3,5458(15)	3,4389(15)
Cg6	Cg4	[4455]	5,242(2)	-1,4134	8,74(18)	52,7	44,5	3,7372(15)	3,1765(16)
Cg7	Cg2	[4565]	4,669(2)	11,1606	55,79(17)	41,2	21,3	4,3499(14)	3,5130(14)
Cg7	Cg3	[1565]	5,855(2)	13,43	88,28(17)	36,2	76	1,4167(14)	4,7268(15)
Cg7	Cg4	[1565]	5,440(2)	12,4531	88,05(17)	16,8	73,2	1,5723(14)	5,2081(16)
Cg7	Cg5	[4555]	5,673(2)	11,7409	84,91(17)	16,8	74,8	1,4922(14)	5,4314(15)
Cg7	Cg6	[4555]	5,094(2)	11,7256	83,76(17)	17,5	71,8	1,5926(14)	4,8587(15)
Cg8	Cg2	[4565]	4,893(2)	11,1606	55,89(18)	44,2	20	4,5990(15)	3,5063(14)
Cg8	Cg5	[4555]	5,527(2)	11,7409	84,74(17)	11,6	77	1,2400(15)	5,4145(15)
Cg8	Cg6	[4555]	5,995(2)	11,7256	83,59(18)	33,7	77,1	1,3389(15)	4,9862(15)

[4465]	-1/2+X,1-Y,Z
[3654]	3/2-X,Y,-1/2+Z
[1565]	X,1+Y,Z
[1545]	X,-1+Y,Z
[4555]	1/2+X,-Y,Z
[4455]	-1/2+X,-Y,Z
[4565]	1/2+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
C25-H25	Cg7	[4455]	2,95	-2,58	28,94	148	3,789(4)	76
C51-H51	Cg5	[1565]	2,76	2,73	8,22	118	3,312(4)	35
C54-H54A	Cg3	[1565]	2,98	-2,92	11,53	121	3,583(4)	40

[4455]	-1/2+X,-Y,Z
[1565]	X,1+Y,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
C15-F5	Cg1	[2665]	3,471(7)	-3,123	25,87	136,3(4)	4,566(5)	20,58
C29-F7	Cg8	[3654]	3,048(3)	3,047	1,45	127,0(2)	3,991(4)	35,89
C29-F9	Cg2	[1555]	3,863(3)	3,38	28,98	97,7(2)	4,250(4)	34,83

[2665]	1-X,1-Y,1/2+Z
[3654]	3/2-X,Y,-1/2+Z
[1555]	X,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	0,39767(7)	0,45343(14)	0,31004(8)
Cg2	0,49854(8)	0,66617(12)	0,44674(8)
Cg3	0,70763(7)	-0,05347(12)	0,51533(8)
Cg4	0,76853(8)	-0,07812(13)	0,62182(8)
Cg5	0,37213(7)	-0,03713(12)	0,47400(8)
Cg6	0,30340(8)	-0,14042(12)	0,39233(8)
Cg7	0,80848(7)	0,48717(12)	0,54508(7)
Cg8	0,85941(8)	0,40455(13)	0,64644(8)

Table S7. Non-coordinative interactions in 5.

6-Membered Ring (1)	N1	-->	C43	-->	C44	-->	C45	-->	C46	-->	C47	-->								
6-Membered Ring (2)	N2	-->	C48	-->	C49	-->	C50	-->	C51	-->	C52	-->								
6-Membered Ring (3)	C5	-->	C6	-->	C7	-->	C12	-->	C13	-->	C14	-->								
6-Membered Ring (4)	C7	-->	C8	-->	C9	-->	C10	-->	C11	-->	C12	-->								
6-Membered Ring (5)	C19	-->	C20	-->	C21	-->	C26	-->	C27	-->	C28	-->								
6-Membered Ring (6)	C21	-->	C22	-->	C23	-->	C24	-->	C25	-->	C26	-->								
6-Membered Ring (7)	C33	-->	C34	-->	C35	-->	C40	-->	C41	-->	C42	-->								
6-Membered Ring (8)	C35	-->	C36	-->	C37	-->	C38	-->	C39	-->	C40	-->								
10-Membered Ring (9)	C5	-->	C6	-->	C7	-->	C8	-->	C9	-->	C10	-->	C11	-->	C12	-->	C13	-->	C14	-->
10-Membered Ring (10)	C19	-->	C20	-->	C21	-->	C22	-->	C23	-->	C24	-->	C25	-->	C26	-->	C27	-->	C28	-->
10-Membered Ring (11)	C33	-->	C34	-->	C35	-->	C36	-->	C37	-->	C38	-->	C39	-->	C40	-->	C41	-->	C42	-->

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.)
- Slippage = Distance between Cg(I) and Perpendicular Projection 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	[2655]	3,6878(11)	-2,9622	8,72(9)	27,5	20,3	3,4586(8)	3,2714(8)
Cg1	Cg6	[2655]	4,2954(12)	-3,2437	12,55(10)	30,7	38,9	3,3441(8)	3,6928(9)
Cg1	Cg8	[2655]	5,6028(12)	6,3688	79,64(10)	29,3	82,5	0,7277(8)	4,8864(9)
Cg1	Cg10	[2655]	3,8201(10)	-3,0445	10,59(8)	24	25	3,4633(8)	3,4906(7)
Cg1	Cg11	[2655]	5,8378(11)	6,7962	80,81(8)	39,3	81,3	0,8783(8)	4,5154(7)
Cg2	Cg3	[1555]	4,9124(11)	0,2704	61,43(10)	8,1	68,4	1,8093(8)	4,8640(8)
Cg2	Cg4	[1555]	5,5595(12)	0,7828	62,76(10)	23,1	72,4	1,6784(8)	5,1132(9)
Cg2	Cg5	[2655]	4,7618(11)	-2,9622	14,58(9)	43,5	55,9	2,6696(8)	3,4558(8)
Cg2	Cg7	[1555]	5,3378(12)	6,1495	63,24(10)	23,5	39,8	4,1015(8)	4,8933(8)
Cg2	Cg7	[2655]	5,8847(12)	7,267	76,67(10)	46,1	57,5	3,1636(8)	4,0824(8)
Cg2	Cg9	[1555]	5,1031(11)	0,5007	62,07(8)	12,1	69,8	1,7651(8)	4,9902(7)
Cg2	Cg10	[2655]	5,7990(11)	-3,0445	16,94(8)	48,8	64,5	2,4948(8)	3,8189(7)
Cg2	Cg11	[1555]	5,6510(11)	6,2483	62,06(8)	23,5	42,3	4,1784(8)	5,1835(7)
Cg3	Cg3	[3666]	3,6685(12)	3,1596	0,00(10)	20,8	20,8	3,4300(8)	3,4300(8)
Cg3	Cg4	[3666]	5,0530(13)	2,7474	1,90(10)	47,7	46,2	3,4973(8)	3,3992(10)
Cg3	Cg7	[2655]	3,7701(12)	7,267	15,45(10)	18,6	11,4	3,6963(9)	3,5741(9)
Cg3	Cg8	[2655]	4,0514(13)	6,3688	13,64(10)	35,6	24,4	3,6900(9)	3,2926(9)
Cg3	Cg9	[3666]	4,2405(11)	2,9409	0,93(8)	36,4	35,7	3,4445(8)	3,4115(7)
Cg3	Cg11	[2655]	3,7140(11)	6,7962	14,50(8)	22,5	8,6	3,6719(9)	3,4303(7)
Cg4	Cg3	[3666]	5,0530(13)	3,1596	1,90(10)	46,2	47,7	3,3992(10)	3,4974(8)
Cg4	Cg7	[2655]	4,1323(13)	7,267	14,46(11)	30	24,3	3,7672(10)	3,5772(9)
Cg4	Cg8	[2655]	5,5315(13)	6,3688	13,04(11)	54	45,5	3,8767(10)	3,2498(9)
Cg4	Cg11	[2655]	4,7241(12)	6,7962	13,69(9)	43,8	36,4	3,8029(10)	3,4104(7)

Cg5	Cg1	[2645]	3,6878(11)	-4,1629	8,72(9)	20,3	27,5	3,2713(8)	3,4588(8)
Cg5	Cg2	[2645]	4,7619(11)	-5,1016	14,58(9)	55,9	43,5	3,4557(8)	2,6697(8)
Cg5	Cg3	[3666]	5,9585(12)	3,1596	48,57(10)	49,3	82,3	0,8019(9)	3,8822(8)
Cg5	Cg7	[4555]	5,9756(12)	3,4431	63,77(10)	18,6	76,3	1,4118(9)	5,6650(8)
Cg5	Cg8	[4555]	4,6089(12)	4,2899	62,21(10)	11,8	70,7	1,5214(9)	4,5118(9)
Cg5	Cg11	[4555]	5,1946(11)	3,8457	63,02(8)	11,6	73,9	1,4403(9)	5,0879(7)
Cg6	Cg1	[2645]	4,2956(12)	-4,1629	12,55(10)	38,9	30,7	3,6929(9)	3,3442(8)
Cg6	Cg8	[4555]	4,7836(13)	4,2899	60,51(11)	19,4	71,6	1,5060(10)	4,5130(9)
Cg6	Cg11	[4555]	5,7862(11)	3,8457	61,17(9)	26,9	75	1,4928(10)	5,1622(7)
Cg7	Cg2	[1555]	5,3379(12)	7,1189	63,24(10)	39,8	23,5	4,8933(8)	4,1015(8)
Cg7	Cg2	[2645]	5,8847(12)	-5,1016	76,67(10)	57,5	46,1	4,0824(8)	3,1637(8)
Cg7	Cg3	[2645]	3,7700(12)	2,0352	15,45(10)	11,4	18,6	3,5741(9)	3,6962(9)
Cg7	Cg4	[2645]	4,1323(13)	1,946	14,46(11)	24,3	30	3,5772(9)	3,7672(10)
Cg7	Cg5	[2655]	4,9800(13)	-2,9622	63,77(10)	30,5	65,8	2,0397(8)	4,2928(9)
Cg7	Cg9	[2645]	3,7651(12)	1,9726	14,95(9)	7,3	17,3	3,5950(9)	3,7347(7)
Cg7	Cg10	[2655]	5,7341(12)	-3,0445	62,74(9)	40,6	67,4	2,2036(8)	4,3507(7)
Cg8	Cg3	[2645]	4,0514(13)	2,0352	13,64(10)	24,4	35,6	3,2925(9)	3,6899(9)
Cg8	Cg4	[2645]	5,5315(13)	1,946	13,04(11)	45,5	54	3,2498(9)	3,8767(10)
Cg8	Cg9	[2645]	4,6941(12)	1,9726	13,32(9)	36,2	45,5	3,2908(9)	3,7863(7)
Cg9	Cg3	[3666]	4,2407(11)	3,1596	0,93(8)	35,7	36,4	3,4116(7)	3,4445(8)
Cg9	Cg7	[2655]	3,7650(12)	7,267	14,95(9)	17,3	7,3	3,7346(7)	3,5950(9)
Cg9	Cg8	[2655]	4,6940(12)	6,3688	13,32(9)	45,5	36,2	3,7862(7)	3,2908(9)
Cg9	Cg9	[3666]	5,0487(10)	2,9409	0,03(7)	47	47	3,4417(7)	3,4415(7)
Cg9	Cg11	[2655]	4,0724(10)	6,7962	14,09(7)	32,4	23,3	3,7403(7)	3,4398(7)
Cg10	Cg1	[2645]	3,8202(10)	-4,1629	10,59(8)	25	24	3,4905(7)	3,4634(8)
Cg10	Cg8	[4555]	4,5272(11)	4,2899	61,34(9)	10,1	70,5	1,5095(7)	4,4576(9)
Cg10	Cg11	[4555]	5,3530(10)	3,8457	62,07(6)	18,6	74,1	1,4624(7)	5,0724(7)
Cg11	Cg2	[1555]	5,6511(11)	7,1189	62,06(8)	42,3	23,5	5,1836(7)	4,1783(8)
Cg11	Cg3	[2645]	3,7140(11)	2,0352	14,50(8)	8,6	22,5	3,4302(7)	3,6719(9)
Cg11	Cg4	[2645]	4,7240(12)	1,946	13,69(9)	36,4	43,8	3,4104(7)	3,8029(10)
Cg11	Cg5	[2655]	5,6551(11)	-2,9622	63,02(8)	41,7	62,4	2,6168(7)	4,2256(9)
Cg11	Cg9	[2645]	4,0725(10)	1,9726	14,09(7)	23,3	32,4	3,4398(7)	3,7404(7)

[2655]	1-X,1/2+Y,1/2-Z
[1555]	X,Y,Z
[3666]	1-X,1-Y,1-Z
[2645]	1-X,-1/2+Y,1/2-Z
[4555]	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
C6-H6	Cg2	[1555]	2,87	2,82	10,85	141	3,658(2)	61
C38-H38	Cg6	[4554]	2,7	2,64	12,11	143	3,505(2)	53
C38-H38	Cg10	[4554]	2,7	2,61	15,28	127	3,362(2)	52
C39-H39	Cg5	[4554]	2,82	2,75	12,81	126	3,467(2)	48

[1555]	X,Y,Z
[4554]	X,1/2-Y,-1/2+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
C15-F5	Cg8	[2645]	3,3602(19)	3,168	19,45	144,30(16)	4,500(3)	60,79

[2645]	1-X,-1/2+Y,1/2-Z
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The Cg(I) refer to the Ring Centre-of-Gravity numbers given in () in the Ring-Analysis above.

Cg(I)	x	y	z
Cg1	0,23010(6)	0,62895(6)	0,24362(3)
Cg2	0,53129(6)	0,52807(6)	0,27263(3)
Cg3	0,53036(6)	0,60464(6)	0,46516(3)
Cg4	0,71522(7)	0,63026(7)	0,48050(4)
Cg5	0,66633(6)	0,15999(6)	0,38482(3)
Cg6	0,83734(7)	0,21262(7)	0,42390(4)
Cg7	0,46276(7)	0,34808(6)	0,08356(3)
Cg8	0,64006(7)	0,33366(7)	0,06771(4)
Cg9	0,62281(5)	0,61728(5)	0,47291(3)
Cg10	0,75169(5)	0,18618(5)	0,40468(3)
Cg11	0,55136(5)	0,34062(5)	0,07563(3)

Table S8. Relaxation parameters values for the best fit of χ_M'' and χ_M' vs. frequency using the generalised Debye model for compound **2**.

T (K)	χ_S (cm ³ ·mol ⁻¹)	χ_T (cm ³ ·mol ⁻¹)	τ (s)	α
2.29606	0.02755	0.29478	9.23953E-4	0.17948
2.39807	0.02736	0.28325	8.09901E-4	0.16875
2.54207	0.0266	0.26706	6.5736E-4	0.1529
2.70185	0.02639	0.25234	5.31087E-4	0.13569
2.85219	0.02633	0.23848	4.26354E-4	0.11536
3.00445	0.02657	0.22569	3.42105E-4	0.09469
3.15329	0.02579	0.21509	2.73913E-4	0.0804
3.30222	0.02709	0.2049	2.21347E-4	0.06166
3.44963	0.0272	0.19565	1.79234E-4	0.04921
3.60098	0.02602	0.18754	1.43677E-4	0.03963
3.76045	0.0295	0.18015	1.20913E-4	0.02297
3.90673	0.02632	0.17356	9.57657E-5	0.02538
4.05689	0.02781	0.16717	7.99235E-5	0.01692
4.20239	0.02679	0.16131	6.52605E-5	0.01499
4.36281	0.02941	0.1561	5.58924E-5	0.00433

Table S9. Relaxation parameters values

for the best fit of χ_M'' and χ_M' vs. frequency using the generalised Debye model for compound **4**.

T (K)	χ_S (cm ³ ·mol ⁻¹)	χ_T (cm ³ ·mol ⁻¹)	τ (s)	α
1.8	0.03039	0.31192	8.73052E-4	0.1967
1.9	0.02928	0.29636	7.67258E-4	0.1892
2.0	0.02892	0.28123	6.73516E-4	0.17826
2.1	0.02846	0.26803	5.93904E-4	0.16907
2.3	0.02846	0.24737	4.71799E-4	0.154
2.5	0.0279	0.22795	3.6437E-4	0.13096
2.7	0.02913	0.21148	2.84815E-4	0.10381
2.9	0.02863	0.19738	2.16885E-4	0.08352
3.1	0.02847	0.18523	1.63182E-4	0.06346
3.3	0.03085	0.17401	1.27623E-4	0.03929

Table S10. Relaxation parameters values for the best fit of χ_M'' and χ_M' vs. frequency using the generalised Debye model for compound **5**.

T (K)	χ_s (cm ³ ·mol ⁻¹)	χ_T (cm ³ ·mol ⁻¹)	τ (s)	α
1.79864	0.02137	0.2703	0.00399	0.17531
1.88865	0.02074	0.27084	0.00376	0.18503
2.00725	0.01913	0.26231	0.00325	0.18583
2.09224	0.0188	0.25183	0.00276	0.17437
2.19807	0.01669	0.2542	0.00259	0.18892
2.2963	0.01698	0.24791	0.00218	0.17928
2.39747	0.01633	0.24185	0.00183	0.17102
2.54297	0.01684	0.22759	0.00133	0.14239
2.69744	0.01749	0.214	9.52479E-4	0.11166
2.85596	0.01771	0.20237	6.88583E-4	0.09262
3.00628	0.01773	0.19181	4.99809E-4	0.07115
3.15398	0.01697	0.18209	3.6221E-4	0.05586
3.30182	0.01752	0.17348	2.66954E-4	0.0417
3.45023	0.01831	0.16543	1.99802E-4	0.02615
3.59888	0.01692	0.15943	1.48855E-4	0.02722
3.76099	0.01886	0.15311	1.15559E-4	0.01387
3.90686	0.01697	0.147	8.65863E-5	0.0086
4.05704	0.01714	0.14217	6.7255E-5	0.01414
4.20375	0.02078	0.13723	5.53884E-5	1.30256E-14