Supplementary Materials

Magnetic and Luminescence Properties of 8-Coordinated Pyridyl Adducts of Samarium(III) Complexes Containing 4,4,4-Trifluoro-1-(naphthalen-2-yl)-1,3-butanedionate

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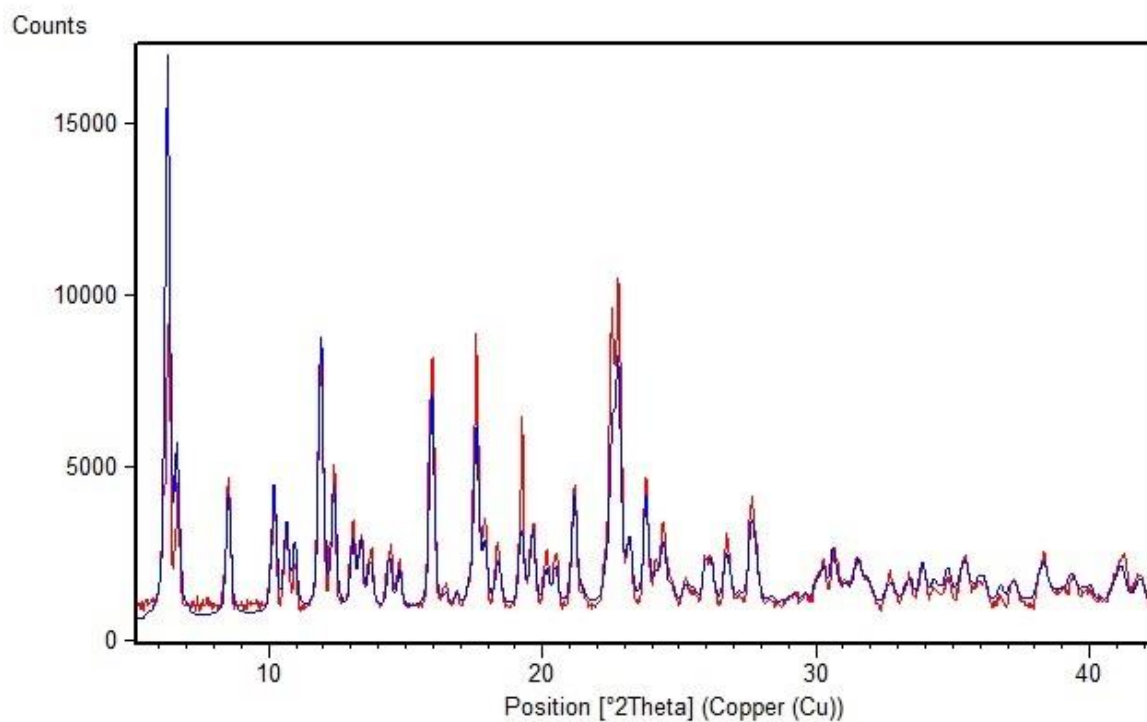
Figure S1. Observed (red) and simulated (blue) PXRD pattern of **1**.
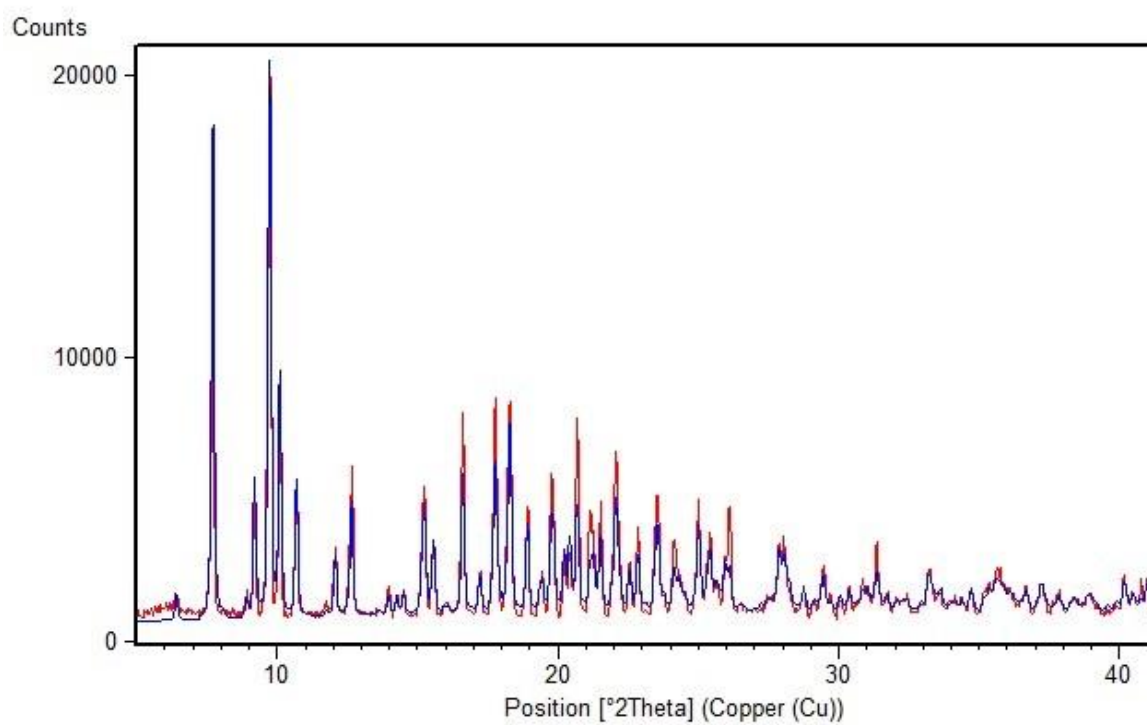

Figure S2. Observed (red) and simulated (blue) PXRD pattern of **2**.
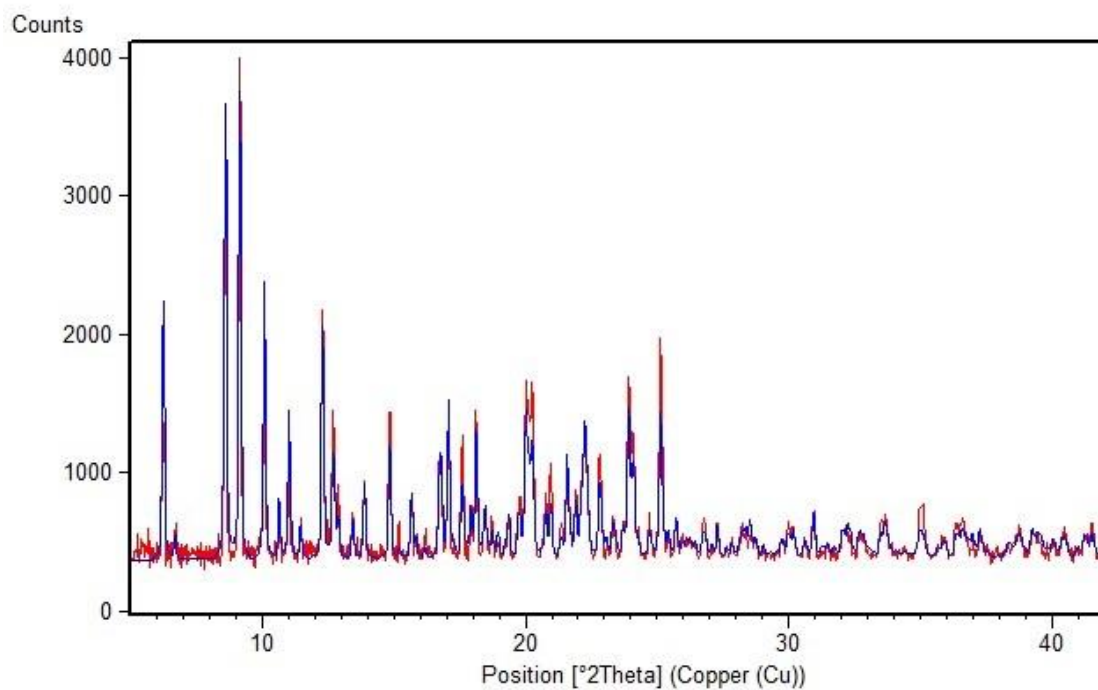
Figure S3. Observed (red) and simulated (blue) PXRD pattern of **3**.
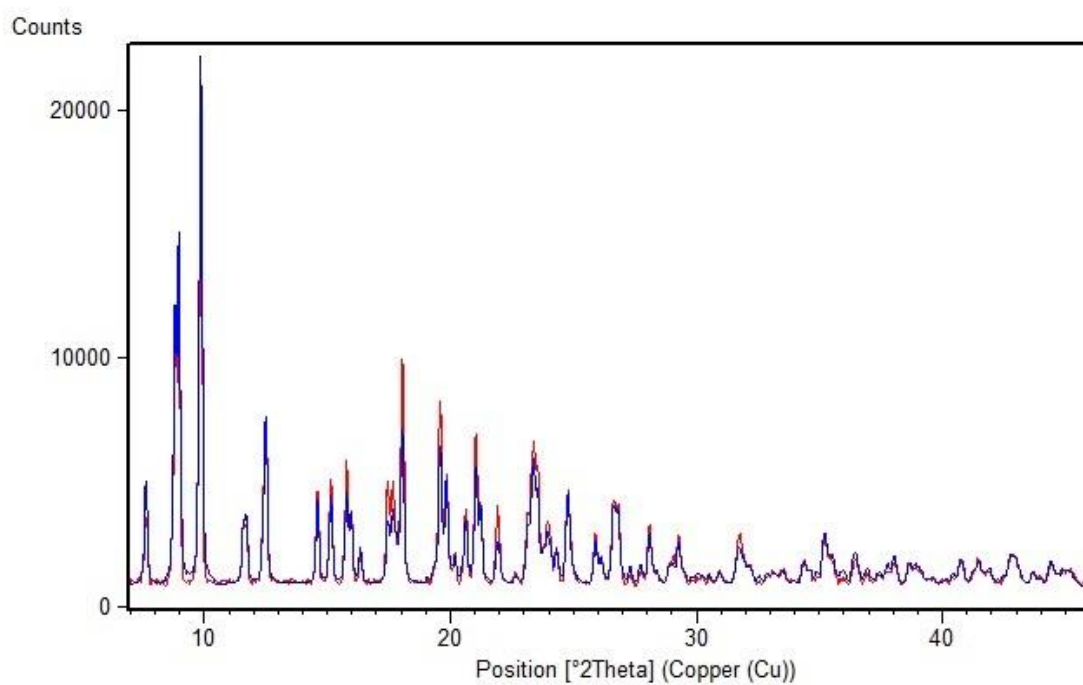

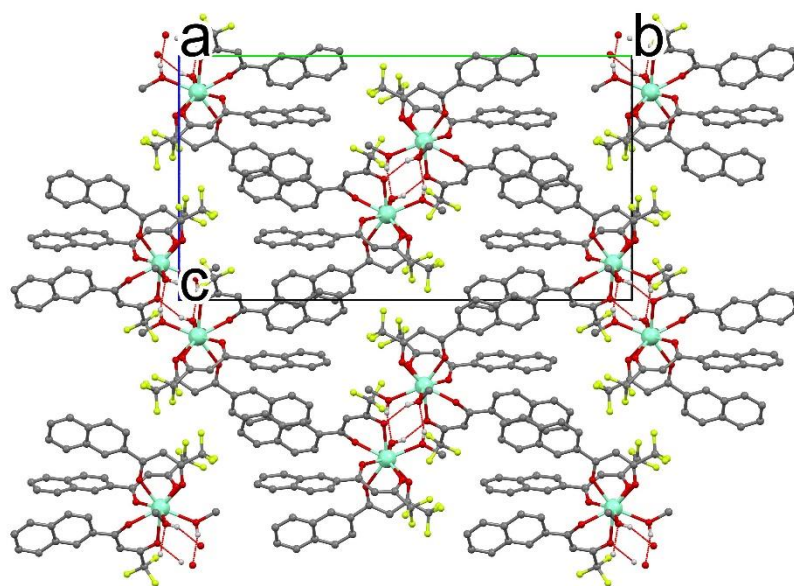**Figure S4**. Observed (red) and simulated (blue) PXRD pattern of **4**.
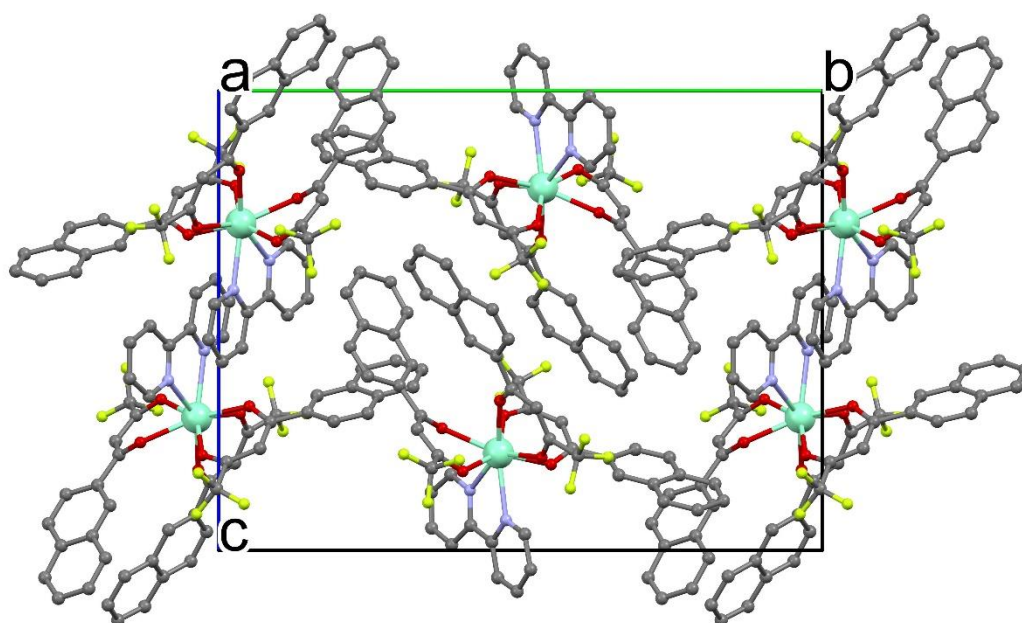
Figure S5. Packing plot of **1**.

Figure S6. Packing plot of **2**.
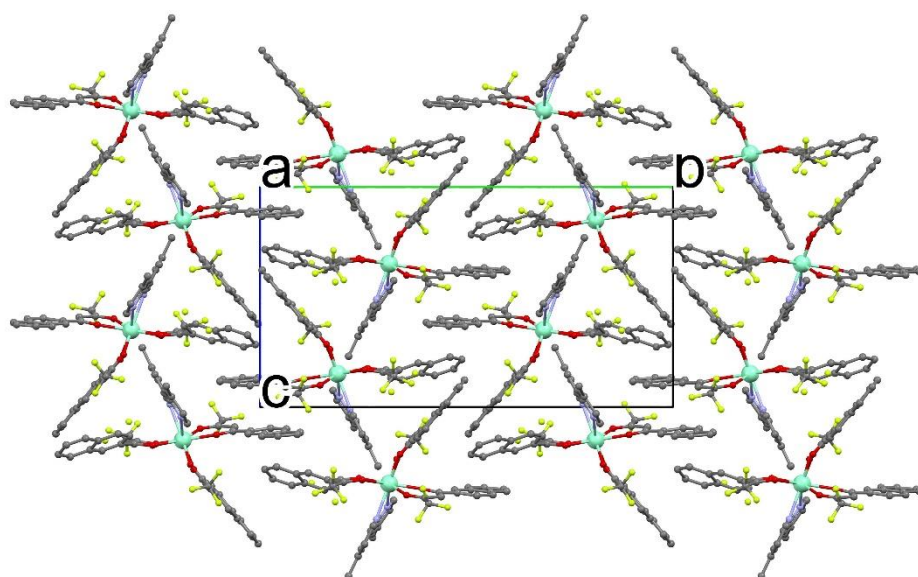
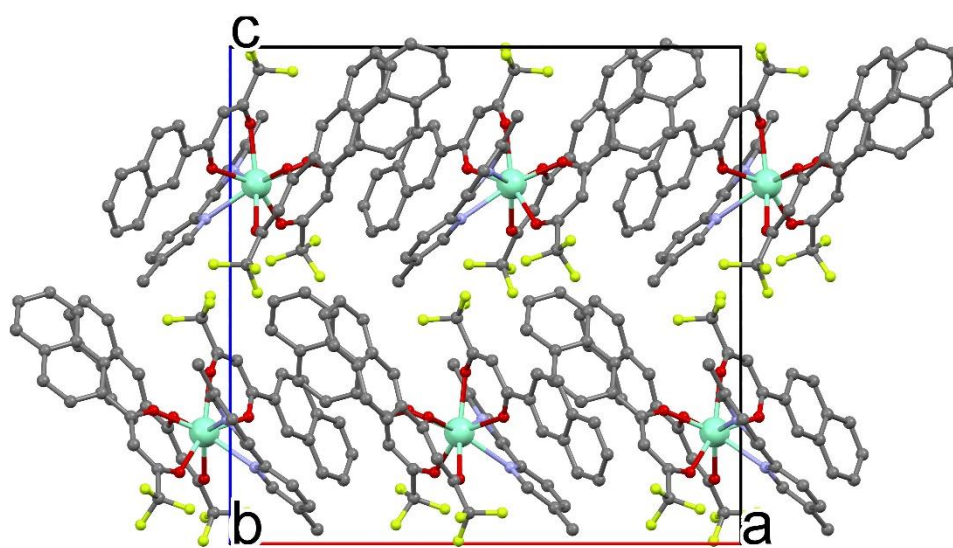**Figure S7**. Packing plot of **3**.

Figure S8. Packing plot of **4**.

Table S1: Noncovalent interactions in **1**.

Definition of aromatic ring systems:

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

Analysis of Short-Ring Interactions:

- Cg(I) = Plane number I (= ring number in () above)

- Cg-Cg = Distance between ring Centroids (Ang.)

Cg3	Cg6	[4565]	3,7185(16)
Cg4	Cg5	[4565]	3,7535(16)
Cg4	Cg6	[4565]	4,0157(16)
Cg5	Cg8	[4564]	4,1695(14)
Cg6	Cg8	[4564]	3,6734(14)
Cg8	Cg9	[4565]	3,7390(13)
Cg9	Cg3	[4564]	4,1561(14)
Cg9	Cg4	[4564]	3,6940(14)

[4564]	X,3/2-Y,-1/2+Z
[4665]	1+X,3/2-Y,1/2+Z

Analysis of X-H...Cg(Pi-Ring) Interactions

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

- X-H..Cg = X-H-Cg angle (degrees)

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

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	X-H..Cg	X..Cg
C8-H8	Cg3	[1555]	2,68	149	3,527(3)

C8-H8	Cg8	[1555]	2,80	137	3,553(3)
C13-H13	Cg6	[1655]	2,85	141	3,638(3)
C13-H13	Cg9	[1655]	2,66	134	3,391(3)
C22-H22	Cg1	[4565]	2,71	142	3,510(3)
C39-H39	Cg2	[4464]	2,88	143	3,682(3)
C39-H39	Cg7	[4464]	2,94	134	3,666(3)

[1555]	X,Y,Z
[1655]	1+X,Y,Z
[4565]	X,3/2-Y,1/2+Z
[4464]	-1+X,3/2-Y,-1/2+Z

Table S2: Noncovalent interactions in **2**.

Definition of aromatic ring systems:

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

- Cg(I) = Plane number I (= ring number in () above)

- Cg-Cg = Distance between ring Centroids (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg
Cg1	Cg2	[3565]	3,867(2)
Cg1	Cg4	[4564]	4,174(2)
Cg5	Cg5	[3666]	3,691(2)

[3565]	-X,1-Y,-Z
[4564]	X,3/2-Y,-1/2+Z
[4565]	X,3/2-Y,1/2+Z
[3666]	1-X,1-Y,1-Z

Analysis of X-H...Cg(Pi-Ring) Interactions

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

- X-H..Cg = X-H-Cg angle (degrees)

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

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	X-H..Cg	X..Cg
C22-H22	Cg3	[1555]	2,76	145	3,574(4)
C22-H22	Cg9	[1555]	2,64	159	3,546(4)
C37-H37	Cg10	[2645]	2,87	131	3,563(4)
C38-H38	Cg5	[2645]	2,84	135	3,579(4)

[1555]	X,Y,Z
[2645]	1-X,-1/2+Y,1/2-Z

Analysis of Y-F...Cg(Pi-Ring) Interactions

Y--F(I)	Cg(J)	[ARU(J)]	F..Cg	Y-F..Cg	Y..Cg
C1-F2	Cg8	[2655]	3,238(3)	133,7(2)	4,276(4)
C1-F2	Cg11	[2655]	3,457(2)	151,6(2)	4,680(4)

[2655]	1-X,1/2+Y,1/2-Z

Table S3: Noncovalent interactions in **3**.

Definition of aromatic ring systems:

6-Membered Ring (2) N2   --> C48   --> C49   --> C50   --> C51   --> C52   -->

6-Membered Ring (5) C19   --> C20   --> C21   --> C26   --> C27   --> C28   -->

6-Membered Ring (6) C21   --> C22   --> C23   --> C24   --> C25   --> C26   -->

Analysis of Short-Ring Interactions

- Cg(I) = Plane number I (= ring number in () above)

- Cg-Cg = Distance between ring Centroids (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg
Cg5	Cg5	[3766]	3,784(2)
Cg5	Cg6	[3766]	3,993(2)
Cg6	Cg5	[3766]	3,993(2)

[3766]	2-X,1-Y,1-Z

Analysis of X-H...Cg(Pi-Ring) Interactions

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

- X-H..Cg = X-H-Cg angle (degrees)

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

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	X-H..Cg	X..Cg
C14-H14	Cg2	[1555]	2,81	159	3,710(4)
C25-H25	Cg2	[3766]	2,90	148	3,748(4)

[1555]	X,Y,Z
[3766]	2-X,1-Y,1-Z

Analysis of Y-F...Cg(Pi-Ring) Interactions

Y--F(I)	Cg(J)	[ARU(J)]	F..Cg	Y-F..Cg	Y..Cg
C1-F3A	Cg6	[2645]	3,88(3)	128,9(14)	4,937(5)

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

Table S4: Noncovalent interactions in **4**.

Definition of aromatic ring systems:

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   -->

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:

- Cg(I) = Plane number I (= ring number in () above)

- Cg-Cg = Distance between ring Centroids (Ang.)

Cg(I)	Cg(J)	[ARU(J)]	Cg-Cg
Cg3	Cg7	[4465]	3,591(3)
Cg3	Cg8	[4465]	3,852(3)
Cg3	Cg11	[4465]	3,516(3)
Cg4	Cg7	[4465]	3,832(4)
Cg7	Cg9	[4565]	3,500(3)
Cg9	Cg7	[4465]	3,500(3)
Cg9	Cg11	[4465]	3,798(3)

[4465]	-1/2+X,1-Y,Z
[4565]	1/2+X,1-Y,Z

Analysis of X-H...Cg(Pi-Ring) Interactions

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

- X-H..Cg = X-H-Cg angle (degrees)

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

X--H(I)	Cg(J)	[ARU(J)]	H..Cg	X-H..Cg	X..Cg
C39-H39	Cg5	[4565]	2,95	146	3,782(6)
C45-H45	Cg7	[1545]	2,78	117	3,330(8)

[4565]	1/2+X,1-Y,Z
[1545]	X,-1+Y,Z

Analysis of Y-F...Cg(Pi-Ring) Interactions

Y--F(I)	Cg(J)	[ARU(J)]	F..Cg	Y-X..Cg	Y..Cg
C15-F5	Cg6	[3654]	3,031(4)	125,6(3)	3,963(6)
C15-F5	Cg10	[3654]	3,352(4)	143,0(3)	4,494(6)
C29-F8	Cg2	[2755]	3,495(5)	137,1(3)	4,573(7)

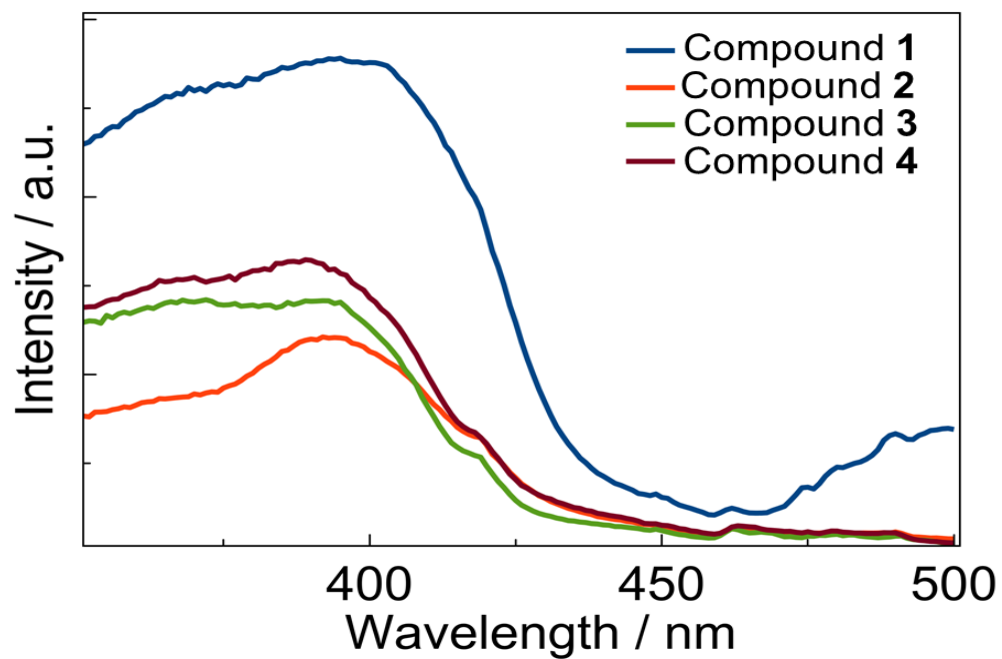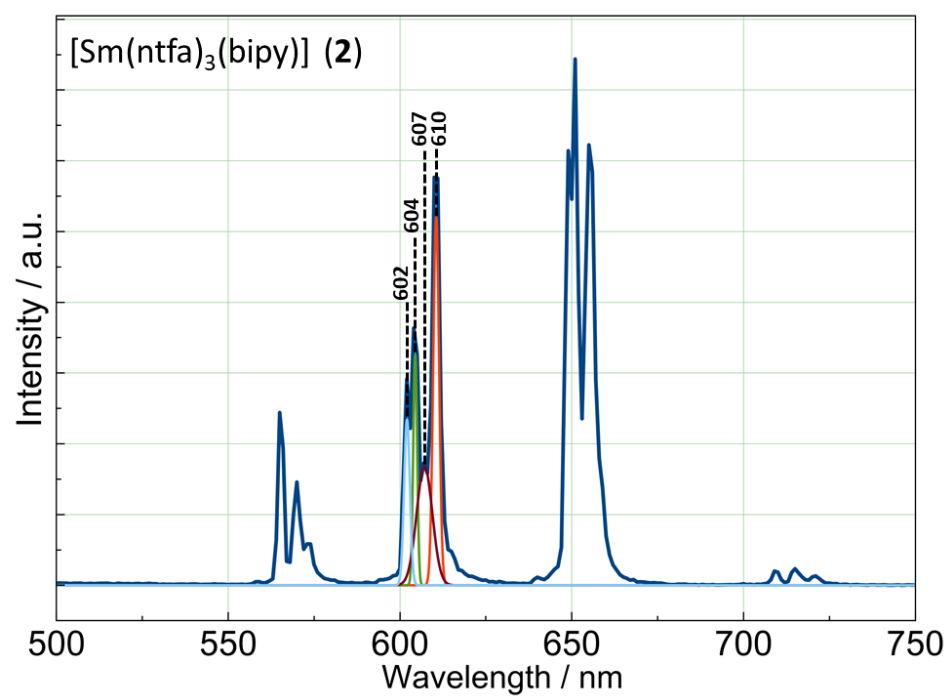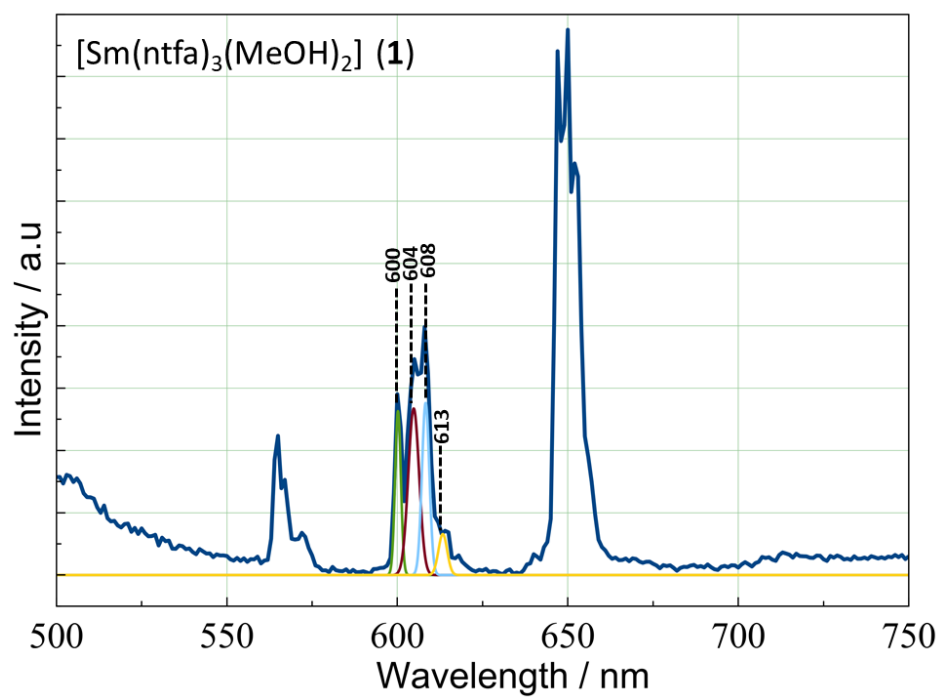| [3654]	3/2-X,Y,-1/2+Z
[2755]	2-X,-Y,1/2+Z

Figure S9. Excitation spectra of compounds **1-4** monitored at the maximum emission wavelength of 649 ± 2 nm ($^{4}G_{5/2} \rightarrow ^{6}H_{9/2}$).
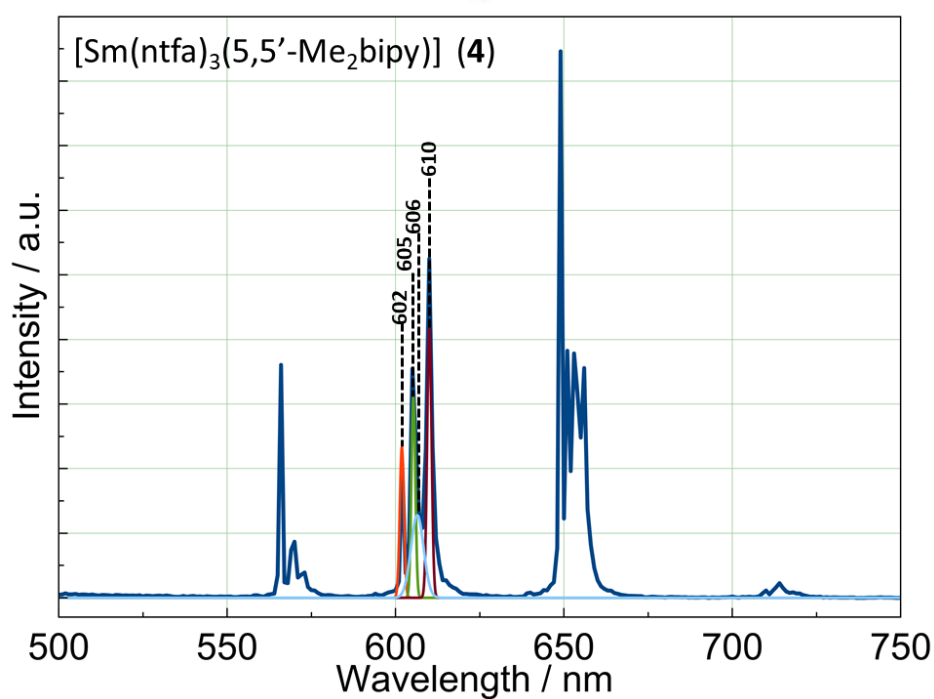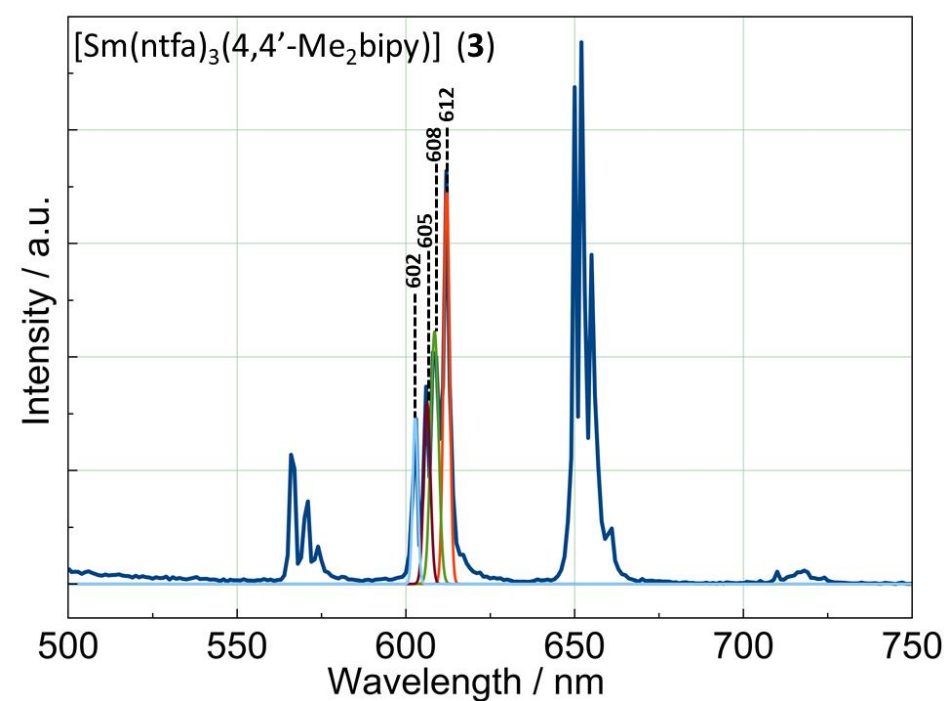
Figure S10. Deconvolution of the magnetic-dipole-allowed band $^4G_{5/2} \rightarrow {}^6H_{7/2}$.