

Electronic Supplementary Information

Solvent and anion effects on the organization of a luminescent [2+2] BODIPY/Ag(I) metallamacrocyclic in the crystalline state

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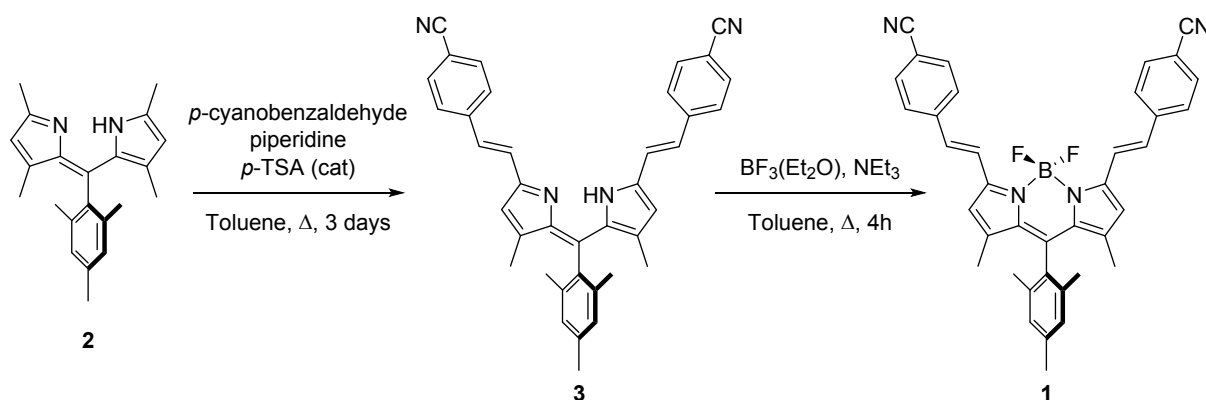
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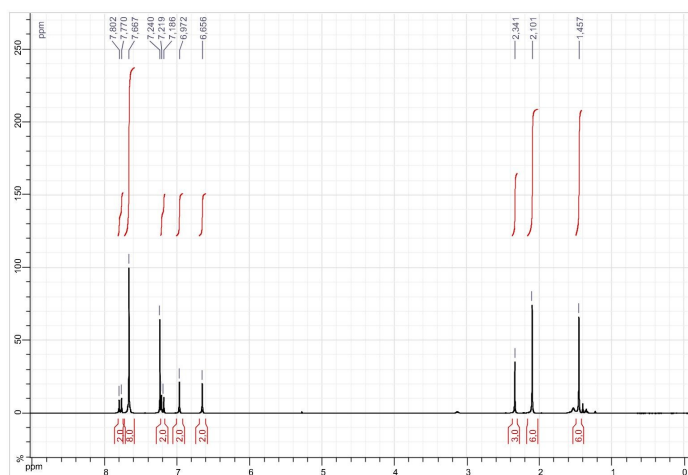


Fig. ESI4 ¹H-NMR spectrum of BODIPY **1** in CDCl₃.

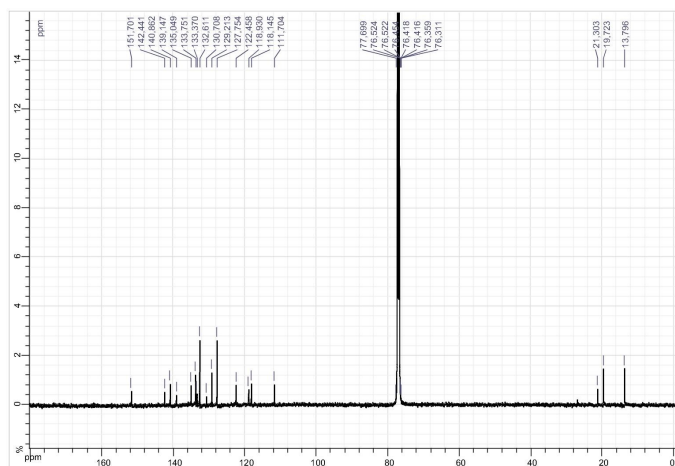


Fig. ESI5 ¹³C-NMR spectrum of BODIPY **1** in CDCl₃.

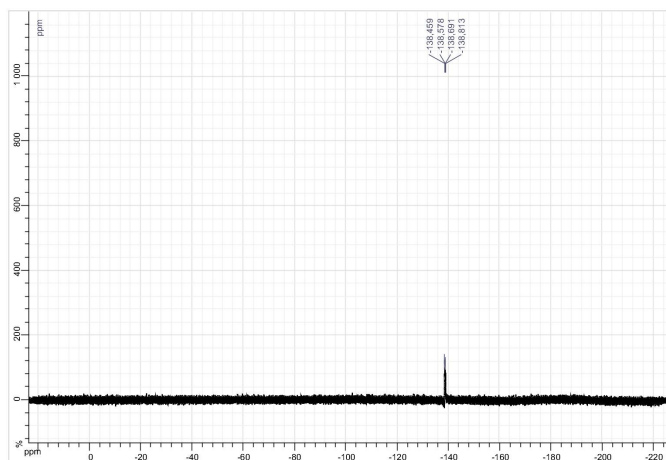


Fig. ESI6 ¹⁹F-NMR spectrum of BODIPY **1** in CDCl₃.

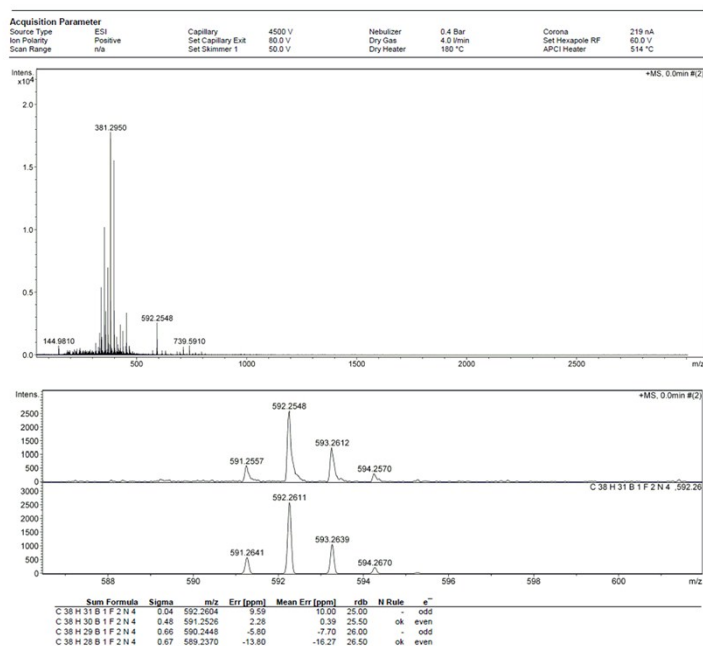


Fig. ESI7 ESI mass spectrum of BODIPY 1

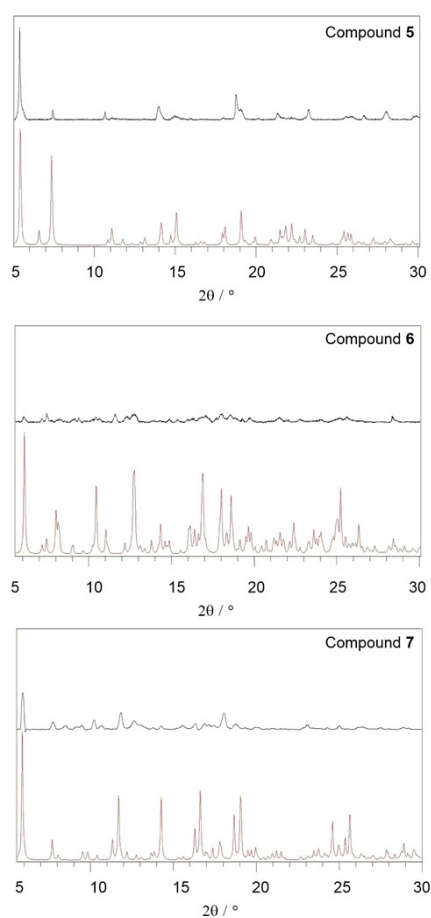


Fig. ESI8 Simulated (a) and experimental (b) PRXD pattern for compounds 5-7 showing the loss of crystallinity of the compounds upon removal from the mother liquor.

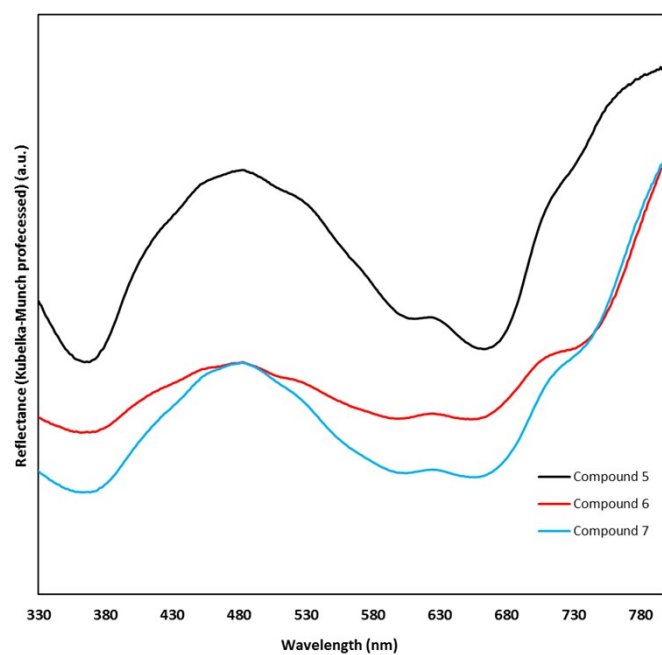


Fig. ESI9 Solid state absorption spectra for compounds **5-7**.

Table ESI1. Crystallographic data for compounds **1** and **3-4**.

	1	3	4
Formula	C ₃₈ H ₃₁ BF ₂ N ₄	C ₃₈ H ₃₂ N ₄	C ₇₈ H ₆₄ Ag ₂ B ₂ Cl ₈ F ₄ N ₈ O ₈
FW	592.48	544.67	1838.33
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	<i>P</i> 2 ₁ / <i>m</i>	<i>P</i> 2 ₁ / <i>n</i>	P-1
<i>a</i> / Å	8.0763(4)	9.9301(8)	10.2626(5)
<i>b</i> / Å	18.6613(11)	23.0445(19)	19.2729(10)
<i>c</i> / Å	10.3428(5)	13.4889(11)	21.5355(11)
α / °			112.493(2)
β / °	91.980(2)	99.355(5)	91.099(2)
γ / °			92.320(2)
<i>V</i> / Å ³	1557.88(14)	3045.7(4)	3929.5(3)
<i>Z</i>	2	4	2
<i>T</i> / K	173(2)	173(2)	173(2)
μ / mm ⁻¹	0.083	0.070	0.841
Refls. coll.	32037	81015	116798
Ind. refls.	4407 (0.0510)	8377 (0.1358)	21506 (0.0774)
(<i>R</i> _{int})			
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>)) ^a	0.0645	0.0657	0.0631
<i>wR</i> ₂ (<i>I</i> > 2σ(<i>I</i>)) ^a	0.1318	0.1454	0.1677
<i>R</i> ₁ (all data) ^a	0.1091	0.1698	0.1646
<i>wR</i> ₂ (all data) ^a	0.1531	0.1871	0.2037
<i>GOF</i>	1.109	0.999	1.055

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|; wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum wF_o^4]^{1/2}$$

Table ESI2. Crystallographic data for compounds **5-7**.

	5	6	7
Formula	C ₇₈ H ₆₄ Ag ₂ B ₂ Cl ₈ F ₄ N ₈	C ₁₇₀ H ₁₅₈ Ag ₄ As ₄ B ₄ Cl ₆ F ₃₂ N ₁₆ O ₈	C ₈₁ H ₇₆ Ag ₂ As ₂ B ₂ F ₁₆ N ₈ O ₂
FW	906.55	4148.21	1884.69
Crystal system	Monoclinic	Triclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1	<i>P</i> 2 ₁
<i>a</i> / Å	18.9253(8)	12.7233 (5)	15.0721(8)
<i>b</i> / Å	8.4818(4)	14.9725(6)	15.6298(9)
<i>c</i> / Å	24.5491(11)	23.8231(10)	17.0390(10)
α / °		90.384(2)	
β / °	101.466(2)	91.008(2)	92.792(2)
γ / °		103.876(2)	
<i>V</i> / Å ³	3862.0(3)	4404.9(3)	4009.2(4)
<i>Z</i>	4	1	2
<i>T</i> / K	173(2)	173(2)	173(2)
μ / mm ⁻¹	0.794	1.369	1.397
Refls. coll.	96266	99759	68702
Ind. refls. (R _{int})	10592 (0.0596)	23829 (0.0608)	22917 (0.0595)
<i>R</i> ₁ (I>2σ(I)) _a	0.1248	0.0862	0.0442
<i>wR</i> ₂ (I>2σ(I)) _a	0.3275	0.2291	0.0916
<i>R</i> ₁ (all data) ^a	0.1842	0.1700	0.0742
<i>wR</i> ₂ (all data) ^a	0.3709	0.2786	0.1037
<i>GOF</i>	1.025	1.037	1.024

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|; wR_2 = [\sum w(F_o^2 - F_c^2)^2 / \sum wF_o^4]^{1/2}$$