

Supporting information

Liquid crystalline and charge transport properties of double-decker cerium phthalocyanine complexes

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Additional Figures and Tables:

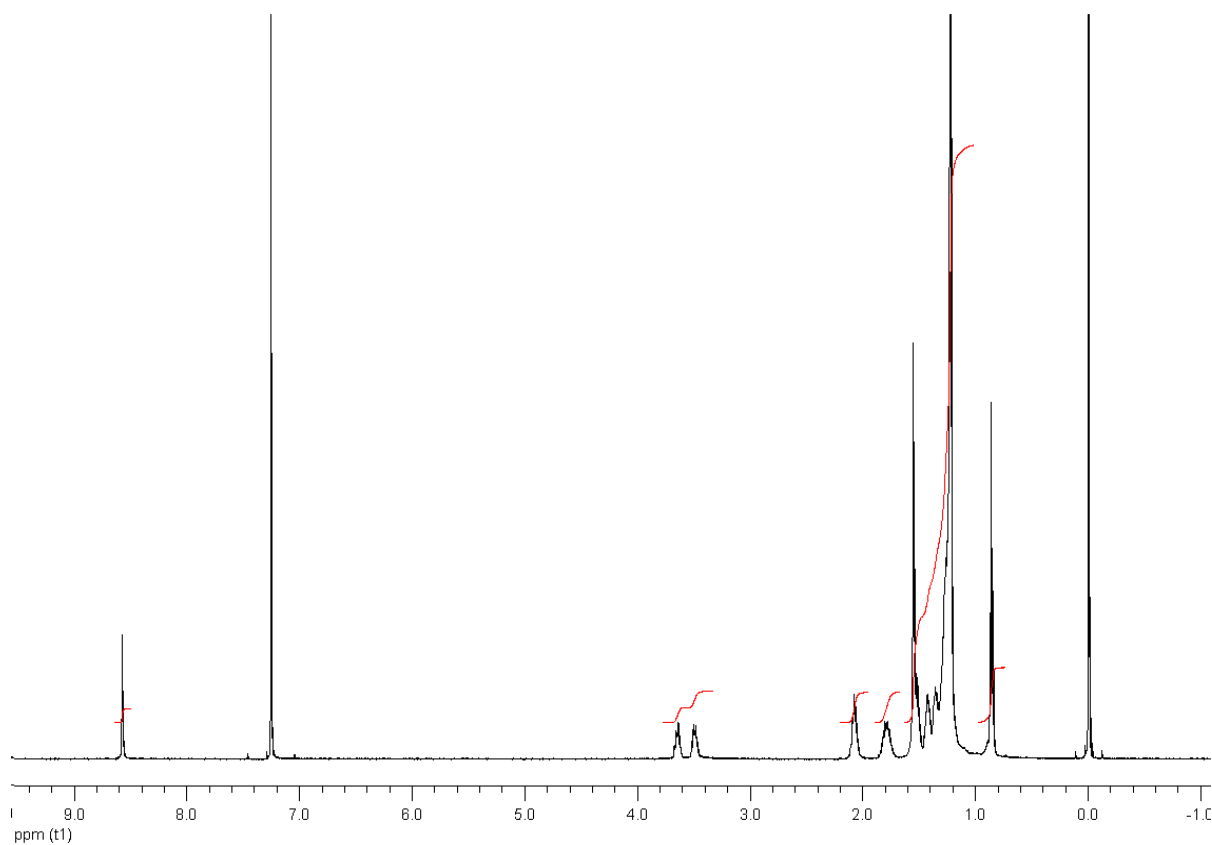


Fig. S1: ¹H NMR spectrum of **3f** in CDCl₃ at 500 MHz.

Table S1. Elemental analyses data for all homologues.

Molecule	Molecular formula	Molecular weight (g.mol ⁻¹)	Elemental analysis; Found % (calculated %)		
			C	H	N
(1a) [(C ₈ H ₁₇) ₈ Pc] ₂ Ce	C ₁₉₂ H ₂₈₈ CeN ₁₆ S ₁₆	3473.69	66.28 (66.39)	8.24 (8.36)	6.21 (6.45)
(1b) [(C ₁₀ H ₂₁) ₈ Pc] ₂ Ce	C ₂₂₄ H ₃₅₂ CeN ₁₆ S ₁₆	3922.55	68.72 (68.59)	9.05 (9.05)	5.67 (5.71)
(1c) [(C ₁₂ H ₂₅) ₈ Pc] ₂ Ce	C ₂₅₆ H ₄₁₆ CeN ₁₆ S ₁₆	4371.42	70.19 (70.34)	9.60 (9.59)	5.10 (5.13)
(1d) [(C ₁₄ H ₂₉) ₈ Pc] ₂ Ce	C ₂₈₈ H ₄₈₀ CeN ₁₆ S ₁₆	4820.29	71.48 (71.76)	9.98 (10.04)	4.64 (4.65)
(1e) [(C ₁₆ H ₃₃) ₈ Pc] ₂ Ce	C ₃₂₀ H ₅₄₄ CeN ₁₆ S ₁₆	5269.15	72.64 (72.94)	10.44 (10.41)	4.17 (4.25)
(1f) [(C ₁₈ H ₃₇) ₈ Pc] ₂ Ce	C ₃₅₂ H ₆₀₈ CeN ₁₆ S ₁₆	5718.02	73.64 (73.94)	10.59 (10.72)	3.62 (3.92)

Table S2. XRD data of cerium phthalocyanine compounds **3a-3f**.

Compound	Temperatures/ °C	Lattice constant/ Å	Spacing / Å		Miller indices (<i>h,k,l</i>)
			Observed	Calculated for Hex	Hex
[(C ₈ H ₁₇ S) ₈ Pc] ₂ Ce (3a)	100	a = 29.6	25.7	25.7	(100)
			14.4	14.8	(110)
			12.4	12.8	(200)
			9.3	9.7	(210)
			8.2	8.8	(300)
			6.8	7.1	(310)
			6.1	6.4	(400)
4.2		Halo of molten alkylthio chains			
[(C ₁₀ H ₂₁ S) ₈ Pc] ₂ Ce (3b)	120	a = 31.7	27.4	27.4	(100)
			15.4	15.8	(110)
			13.3	13.7	(200)
			10.0	10.4	(210)
			8.8	9.1	(300)
			7.3	7.6	(310)
			6.5	6.9	(400)
	4.3		Halo of molten alkylthio chains		
	23	a = 33.5 h = 7.0 c = 3.3	29.0	29.0	(100)
			16.4	16.8	(110)
			14.1	14.5	(200)
			10.6	11.0	(210)
			9.3	9.7	(300)
			8.0	8.1	(310)
7.7			7.3	(400)	
7.0		h			
4.3		Halo of molten alkylthio chains			
3.3		c			
[(C ₁₂ H ₂₅ S) ₈ Pc] ₂ Ce (3c)	160	a = 31.5	27.2	27.2	(100)
			15.7	15.7	(110)
			13.5	13.6	(200)
			10.3	10.3	(210)
			4.6		Halo of molten alkylthio chains
	22	a = 33.1 h = 7.0 c = 3.4	28.7	28.7	(100)
			16.6	16.5	(110)
			14.3	14.3	(200)
			10.9	10.8	(210)
			9.4	9.6	(300)
7.0		h			
4.4		Halo of molten alkylthio chains			
3.4		c			
[(C ₁₄ H ₂₉ S) ₈ Pc] ₂ Ce (3d)	80	a = 35.0	31.2	30.3	(100)
			17.3	17.5	(110)
			15.2	15.2	(200)
			11.9	11.5	(210)
			10.0	10.1	(300)
			8.4	8.4	(310)
			7.5	7.6	(400)
			6.0	6.1	(500)
	4.7		Halo of molten alkylthio chains		
	23	a = 36.3 c = 3.3	32.1	31.4	(100)
			18.4	18.1	(110)
			15.7	15.7	(200)
			11.8	11.9	(210)
			10.5	10.5	(300)
			8.7	8.7	(310)
			7.9	7.9	(400)
			6.8	6.9	(410)
6.3			6.3	(500)	
4.4		Halo of molten alkylthio chains			
4.3		Halo of molten alkylthio chains			
3.3		c			

(Continued)

[(C₁₆H₃₃S)₈Pc]₂Ce (3e)	80	a = 37.4	33.4 18.5 16.2 12.4 10.7 7.9 7.0 4.6	32.4 18.7 16.2 12.2 10.8 8.1 7.1	(100) (110) (200) (210) (300) (400) (410) Halo of molten alkylthio chains
	23	a = 38.1 c = 3.3	33.6 19.1 16.5 10.9 9.3 8.2 7.3 6.8 4.4 4.1 3.3	33.0 19.1 16.5 11.0 9.2 8.3 7.2 6.6	(100) (110) (200) (300) (310) (400) (410) (500) Halo of molten alkylthio chains Halo of molten alkylthio chains c
[(C₁₈H₃₇S)₈Pc]₂Ce (3f)	80	a = 38.6	33.4 19.9 16.4 12.6 11.0 8.1 4.6	33.4 19.3 16.7 12.6 11.1 8.4	(100) (110) (200) (210) (300) (400) Halo of molten alkylthio chains
	25	a = 38.9 c = 3.3	33.7 19.9 16.7 12.7 11.1 9.2 8.3 7.2 6.6 4.2 3.3	33.7 19.5 16.8 12.7 11.2 9.3 8.4 7.4 6.7	(100) (110) (200) (210) (300) (310) (400) (410) (500) Halo of molten alkylthio chains c

²⁰ h: Stacking periodicity between double-decker complexes.

C: Stacking periodicity between single-decker complexes.

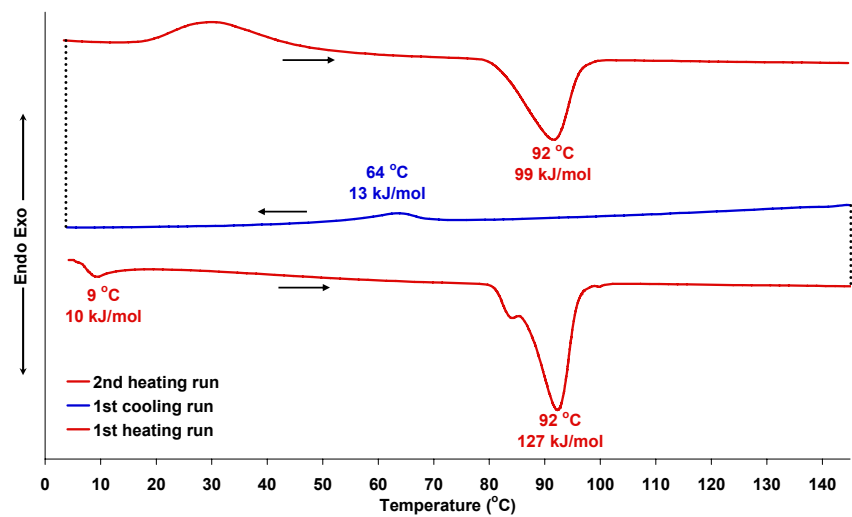
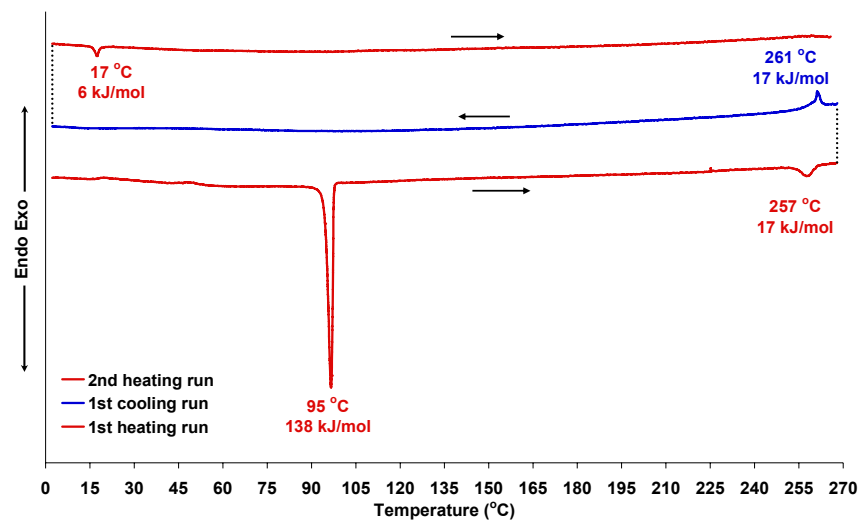


Fig. S2: DSC thermograms of 3a at 1 °C/min.

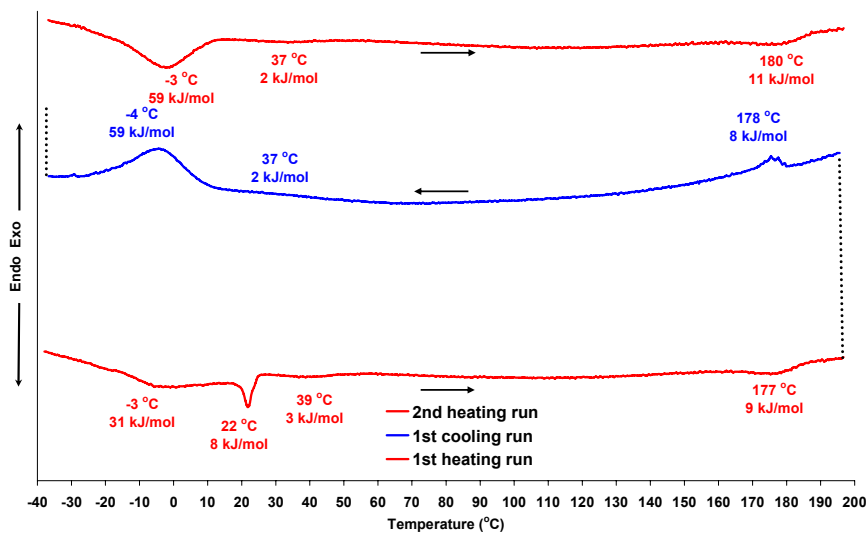


Fig. S3: DSC thermogram of 3c at 1 °C/min.

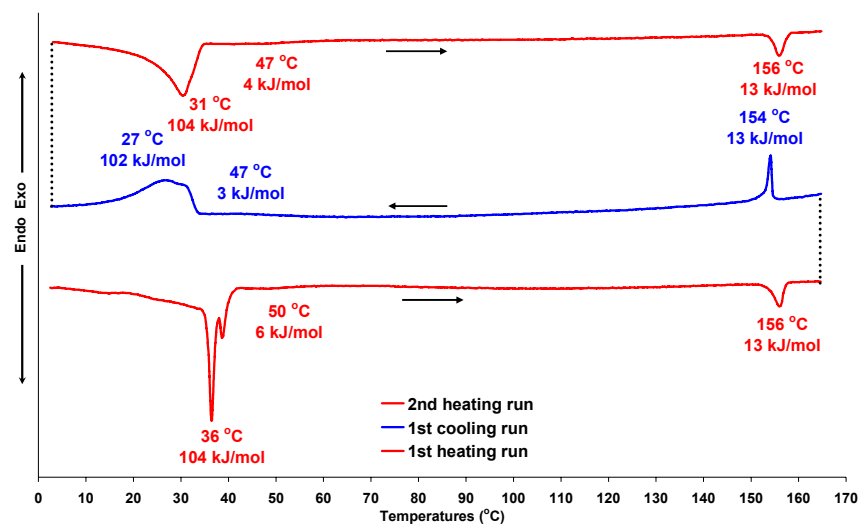


Fig. S4: DSC thermogram of **3d** at 1 °C/min.

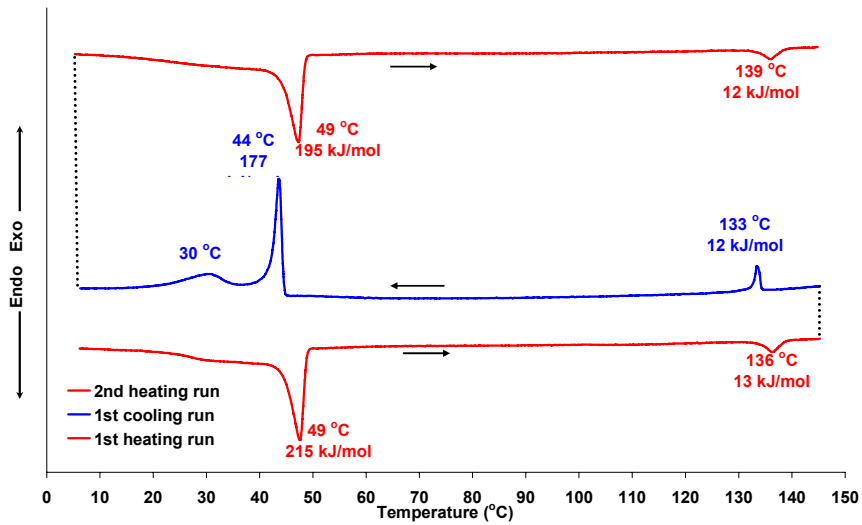


Fig. S5: DSC thermogram of **3e** at 1 °C/min.

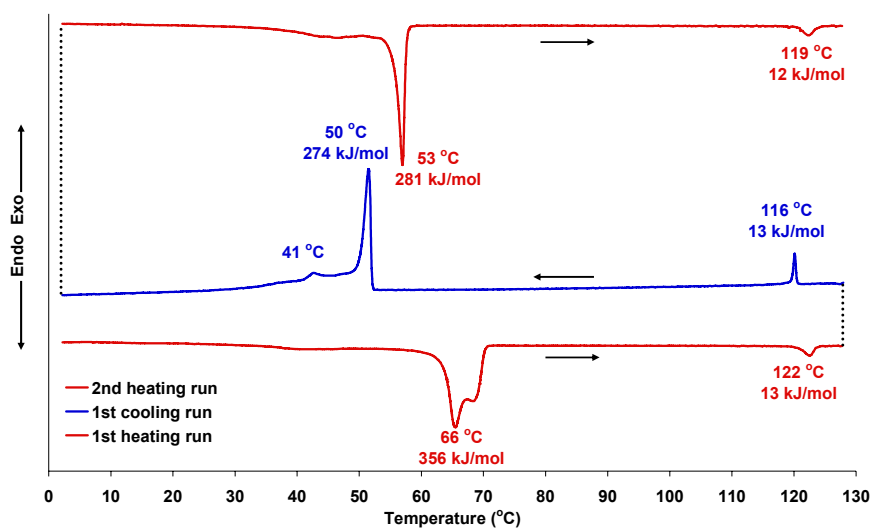


Fig. S6: DSC thermogram of 3f at 1 °C/min.