Electronic Supplementary Material (ESI) for RSC Advances

Electronic Supplementary Information

Solid-state thermo- and photochromism in *N*,*N*′-bis(5-X-salicylidene)diamines (X = H, Br)

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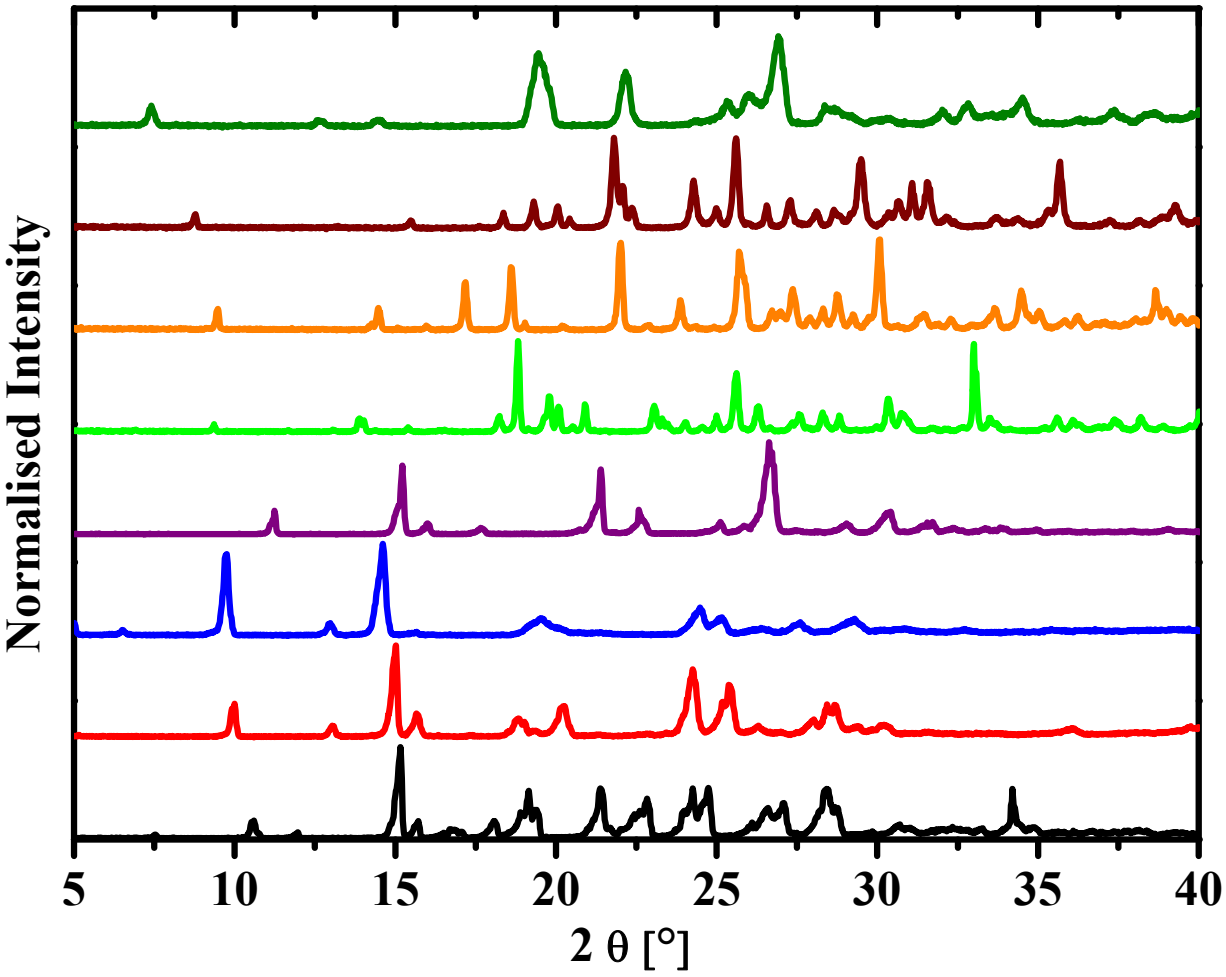

Fig. S1 Powder X-ray diffraction patterns of **1a** (black), **2a** (red), **3a** (blue), **4a** (purple), **1b** (green), **2b** (orange), **3b** (brown) and **4b** (olive).

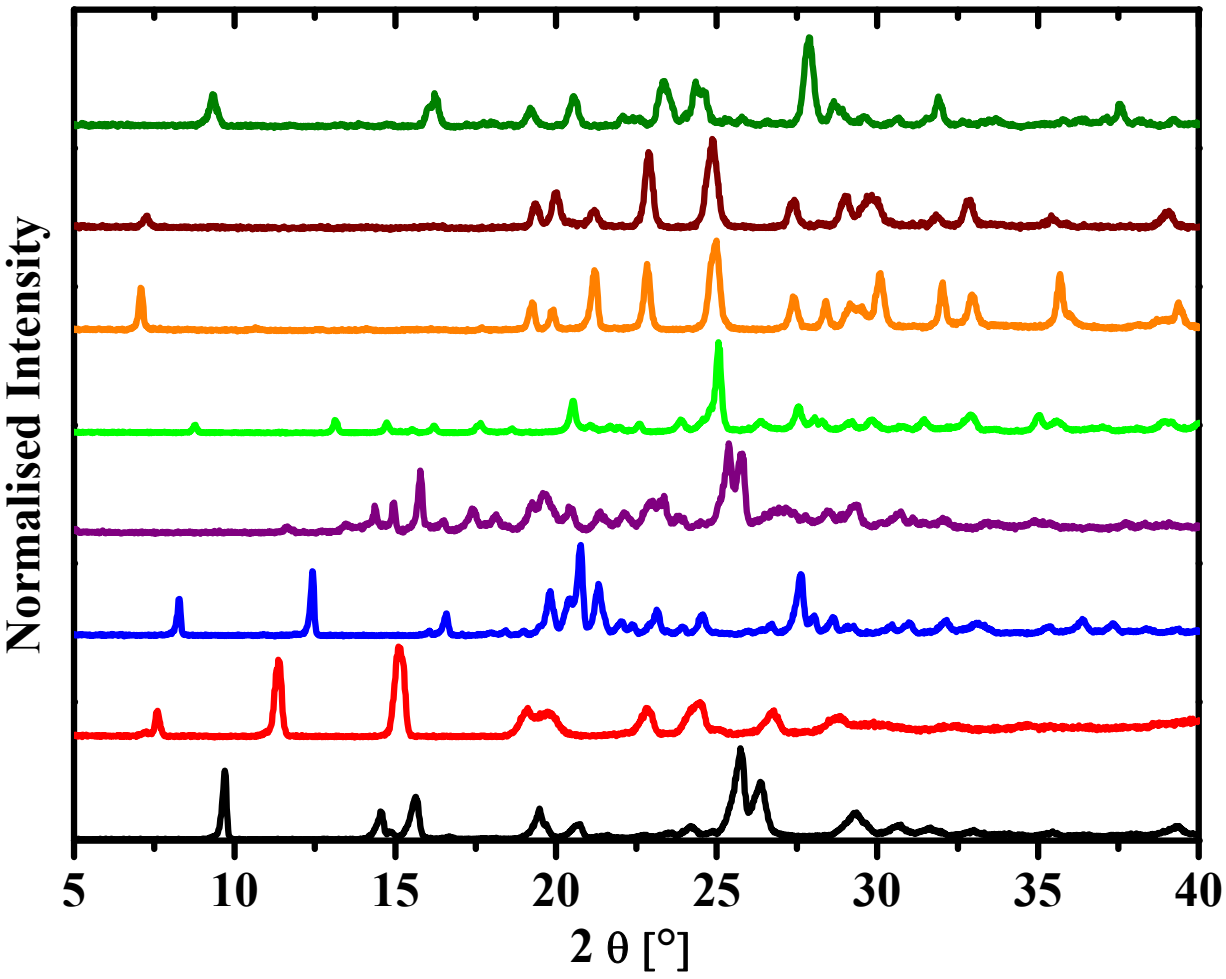

Fig. S2 Powder X-ray diffraction patterns of **5a** (black), **6a** (red), **7a** (blue), **8a** (purple), **5b** (green), **6b** (orange), **7b** (brown) and **8b** (olive).

Table S1 Selected bond lengths (Å) and bond angles (°) for **2a**, **6a**, **7a**, **8a** and **4b**

2a[a]		**6a**[b]		**7a**[c]		**8a**[d]		**4b**[e]	
Bond lengths									
O(15)–C(14)	1.357(3)	O(1)–C(2)	1.342(3)	O(16)–C(15)	1.346(3)	O(18)–C(17)	1.350(3)	O(8)–C(5)	1.347(5)
O(24)–C(23)	1.357(3)	O(31)–C(30)	1.350(3)	O(31)–C(30)	1.352(3)	N(10)–C(7)	1.423(3)	N(10)–N(10)a	1.406(4)
N(7)–C(6)	1.423(3)	N(9)–C(8)	1.273(3)	N(8)–C(5)	1.422(2)	N(10)–C(11)	1.281(3)	N(10)–C(9)	1.259(5)
N(7)–C(8)	1.288(3)	N(9)–C(10)	1.403(3)	N(8)–C(9)	1.276(3)	C(11)–C(12)	1.451(4)	C(4)–C(9)	1.456(5)
N(16)–C(2)	1.436(3)	N(23)–C(20)	1.403(3)	N(23)–C(20)	1.413(3)				
N(16)–C(17)	1.279(3)	N(23)–C(24)	1.302(3)	N(23)–C(24)	1.279(3)				
C(8)–C(9)	1.449(4)	C(7)–C(8)	1.419(3)	C(9)–C(10)	1.447(3)				
C(17)–C(18)	1.450(3)	C(24)–C(25)	1.413(3)	C(24)–C(25)	1.444(3)				
Bond angles									
C(6)–N(7)–C(8)	120.0(2)	C(8)–N(9)–C(10)	121.6(2)	C(5)–N(8)–C(9)	122.57(17)	C(7)–N(10)–C(11)	121.7(2)	N(10)–C(9)–C(4)	121.7(4)
C(2)–N(16)–C(17)	121.7(2)	C(20)–N(23)–C(24)	122.2(2)	C(20)–N(23)–C(24)	123.22(19)				
Torsion angles									
C(3)–C(2)–N(16)–C(17)	–9.8(4)	C(8)–N(9)–C(10)–C(11)	–43.5(2)	C(6)–C(5)–N(8)–C(9)	–4.3(3)	C(11)–N(10)–C(7)–C(8)	17.0(4)	C(9)–N(10)–N(10)a–C(9)a	180.0(3)
C(5)–C(6)–N(7)–C(8)	38.1(3)	C(24)–N(23)–C(20)–C(19)	–41.1(2)	C(19)–C(20)–N(23)–C(24)	–0.8(3)				
Dihedral angles (Φ)									
Cg(1)–Cg(2)	46.53(12)	Cg(1)–Cg(2)	51.64(9)	Cg(1)–Cg(2)	3.22(11)	Cg(1)–Cg(2)	14.53(13)	Cg(1)–Cg(1)	0
Cg(1)–Cg(3)	5.77(13)	Cg(3)–Cg(4)	50.40(9)	Cg(3)–Cg(4)	2.13(11)	Cg(1)–Cg(1)	80.66(10)		
		Cg(2)–Cg(3)	53.72(8)	Cg(1)–Cg(3)	73.63(10)				

[a]Cg(1): C(1)–C(2)–C(3)–C(4)–C(5)–C(6), Cg(2): C(9)–C(10)–C(11)–C(12)–C(13)–C(14), Cg(3): C(18)–C(19)–C(20)–C(21)–C(22)–C(23).

[b]Cg(1): C(2)–C(3)–C(4)–C(5)–C(6)–C(7), Cg(2): C(10)–C(11)–C(12)–C(13)–C(14)–C(15), Cg(3): C(17)–C(18)–C(19)–C(20)–C(21)–C(22), Cg(4): C(25)–C(26)–C(27)–C(28)–C(29)–C30).

[c]Cg(1): C(2)–C(3)–C(4)–C(5)–C(6)–C(7), Cg(2): C(10)–C(11)–C(12)–C(13)–C(14)–C(15), Cg(3): C(17)–C(18)–C(19)–C(20)–C(21)–C(22), Cg(4): C(25)–C(26)–C(27)–C(28)–C(29)–C(30).

[d]Cg(1): C(4)–C(5)–C(6)–C(7)–C(8)–C(9), Cg(2): C(12)–C(13)–C(14)–C(15)–C(16)–C(17).

[e]Cg(1): C(2)–C(3)–C(4)–C(5)–C(6)–C(7).

Table S2 Selected hydrogen bond lengths (Å) and angles (°) for **2a**, **6a**, **7a**, **8a** and **4b**

Compound	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
2a[a]	O(15)–H(15)···N(7)	0.82	1.90	2.627(3)	148
	O(24)–H(24)···N(16)	0.82	1.90	2.629(3)	147
	C(5)–H(5)···O(15)#1	0.93	2.55	3.366(3)	147
6a	O(1)–H(1)···N(9)	0.82	1.87	2.606(3)	148
	O(31)–H(31)···N(23)	0.82	1.88	2.603(3)	147
7a	O(16)–H(16)···N(8)	0.82	1.88	2.605(2)	148
	O(31)–H(31)···N(23)	0.82	1.86	2.587(2)	147
8a[a]	O(18)–H(18)···N(10)	0.80	1.89	2.604(3)	148
	C(5)–H(5)···O(2)#2	0.93	2.59	3.245(3)	128
4b	O(8)–H(8)···N(10)	0.82	1.94	2.656(5)	145

[a]Symmetry transformations used to generate equivalent atoms: #1 x, $-1 + y$, z; #2 $-x$, $1 - y$, $-z$.

Table S3 Selected π···π interactions for **2a**, **6a**, **7a**, **8a** and **4b**

Compound	Cg(*I*)	Cg(*J*)	Cg–Cg (Å)	Dihedral angle (°)	*β* (°)
2a[a]	Cg(1)	Cg(2)	4.7953(15)	46.53(12)	15.77
	Cg(1)	Cg(2)	4.7982(15)	46.53(12)	17.36
	Cg(2)	Cg(1)	4.8277(15)	46.53(12)	20.54
	Cg(2)	Cg(1)	4.7656(15)	46.53(12)	18.80
	Cg(3)	Cg(3)	4.7453(16)	42	19.79
	Cg(3)	Cg(3)	4.8905(16)	42	22.75
6a[b]	Cg(1)	Cg(4)	4.7140(14)	45.56	15.28
	Cg(1)	Cg(4)	4.7214(15)	45.56	16.98
	Cg(2)	Cg(3)	4.7804(12)	57.85	15.57
	Cg(2)	Cg(3)	4.6516(13)	57.85	16.36
	Cg(3)	Cg(2)	4.6636(13)	57.85	16.25
	Cg(3)	Cg(2)	4.7712(12)	57.85	15.19
	Cg(4)	Cg(1)	4.6469(14)	45.56	17.61
	Cg(4)	Cg(1)	4.7849(15)	45.56	17.98
7a[c]	Cg(1)	Cg(3)	4.9959(13)	76.70(10)	10.70
	Cg(1)	Cg(3)	5.0680(13)	76.70(10)	13.51
	Cg(2)	Cg(2)	5.2968(14)	0	56.04
	Cg(2)	Cg(4)	5.1328(15)	76.44(12)	7.44
	Cg(2)	Cg(4)	4.9492(15)	76.44(12)	17.48
	Cg(3)	Cg(1)	5.1278(13)	73.63(10)	67.60
	Cg(3)	Cg(1)	5.2384(13)	76.70(10)	19.81
	Cg(4)	Cg(2)	5.2475(15)	76.44(12	16.65
8a[d]	Cg(1)	Cg(1)	4.9252(19)	81	49.68
	Cg(1)	Cg(2)	4.679(2)	14.53(13)	45.77
	Cg(2)	Cg(1)	4.678(2)	14.53(13)	41.85
4b[e]	Cg(1)	Cg(1)	3.756(2)	0	23.68
	Cg(1)	Cg(1)	3.768(2)	0	12.15

[a]Cg(1): C(1)–C(2)–C(3)–C(4)–C(5)–C(6), Cg(2): C(9)–C(10)–C(11)–C(12)–C(13)–C(14), Cg(3): C(18)–C(19)–C(20)–C(21)–C(22)–C(23).
[b]Cg(1): C(2)–C(3)–C(4)–C(5)–C(6)–C(7), Cg(2): C(10)–C(11)–C(12)–C(13)–C(14)–C(15), Cg(3): C(17)–C(18)–C(19)–C(20)–C(21)–C(22), Cg(4): C(25)–C(26)–C(27)–C(28)–C(29)–C30).
[c]Cg(1): C(2)–C(3)–C(4)–C(5)–C(6)–C(7), Cg(2): C(10)–C(11)–C(12)–C(13)–C(14)–C(15), Cg(3): C(17)–C(18)–C(19)–C(20)–C(21)–C(22), Cg(4): C(25)–C(26)–C(27)–C(28)–C(29)–C(30).
[d]Cg(1): C(4)–C(5)–C(6)–C(7)–C(8)–C(9), Cg(2): C(12)–C(13)–C(14)–C(15)–C(16)–C(17).
[e]Cg(1): C(2)–C(3)–C(4)–C(5)–C(6)–C(7).