Electronic Supplementary Information

Solid state photochromism and thermochromism in *N*-salicylidene pyrene derivatives

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Table S1 Selected bond lengths (Å) and bond angles (°) for **2**

Bond lengths					
Cl(1)–C(25)	1.741(3)	C(5)–C(6)	1.432(4)	C(13)–C(14)	1.390(4)
O(1)–C(22)	1.337(3)	C(6)–C(7)	1.391(4)	C(13)–C(17)	1.420(4)
N(1)–C(1)	1.281(4)	C(6)–C(16)	1.423(4)	C(14)–C(15)	1.377(4)
N(1)–C(2)	1.410(4)	C(7)–C(8)	1.385(5)	C(16)–C(17)	1.422(4)
C(1)–C(21)	1.450(4)	C(8)–C(9)	1.374(4)	C(21)–C(22)	1.420(4)
C(2)–C(3)	1.408(4)	C(9)–C(10)	1.400(4)	C(21)–C(26)	1.388(4)
C(2)–C(15)	1.402(4)	C(10)–C(11)	1.434(4)	C(22)–C(23)	1.381(4)
C(3)–C(4)	1.437(4)	C(10)–C(16)	1.420(4)	C(23)–C(24)	1.393(4)
C(3)–C(17)	1.424(4)	C(11)–C(12)	1.341(5)	C(24)–C(25)	1.387(4)
C(4)–C(5)	1.346(4)	C(12)–C(13)	1.435(4)	C(25)–C(26)	1.378(4)
Bond angles					
C(1)–N(1)–C(2)	120.9(2)	C(8)–C(9)–C(10)	121.3(3)	C(16)–C(6)–C(5)	118.2(2)
N(1)–C(1)–C(21)	122.0(3)	C(9)–C(8)–C(7)	120.4(3)	C(16)–C(10)–C(11)	118.9(3)
C(3)–C(2)–N(1)	118.6(2)	C(9)–C(10)–C(11)	122.6(3)	C(16)–C(17)–C(3)	119.9(2)
C(15)–C(2)–N(1)	121.4(3)	C(9)–C(10)–C(16)	118.6(3)	C(17)–C(3)–C(4)	118.5(3)
O(1)–C(22)–C(21)	121.6(3)	C(10)–C(16)–C(6)	119.7(3)	C(17)–C(13)–C(12)	118.6(3)
O(1)–C(22)–C(23)	119.0(2)	C(10)–C(16)–C(17)	120.0(2)	C(17)–C(16)–C(6)	120.3(2)
C(24)–C(25)–Cl(1)	118.9(2)	C(11)–C(12)–C(13)	121.9(3)	C(22)–C(21)–C(1)	120.7(2)
C(26)–C(25)–Cl(1)	120.2(2)	C(12)–C(11)–C(10)	121.0(3)	C(22)–C(23)–C(24)	120.9(3)
C(2)–C(3)–C(4)	122.9(2)	C(13)–C(17)–C(3)	120.4(3)	C(23)–C(22)–C(21)	119.4(2)
C(2)–C(3)–C(17)	118.7(2)	C(13)–C(17)–C(16)	119.7(2)	C(25)–C(24)–C(23)	119.1(3)
C(4)–C(5)–C(6)	122.0(2)	C(14)–C(13)–C(12)	122.4(2)	C(25)–C(26)–C(21)	120.5(3)
C(5)–C(4)–C(3)	121.2(3)	C(14)–C(13)–C(17)	119.0(3)	C(26)–C(21)–C(1)	120.2(2)
C(7)–C(6)–C(5)	122.8(2)	C(14)–C(15)–C(2)	121.1(3)	C(26)–C(21)–C(22)	119.1(3)
C(7)–C(6)–C(16)	119.1(2)	C(15)–C(2)–C(3)	119.8(3)	C(26)–C(25)–C(24)	120.9(3)
C(8)–C(7)–C(6)	120.9(3)	C(15)–C(14)–C(13)	121.0(2)		
Torsion angles					
C(1)–N(1)–C(2)–C(3)	–149.8(3)	C(1)–N(1)–C(2)–C(15)	35.2(5)		

Table S2 Selected bond lengths (Å) and bond angles (°) for **3**

Bond lengths					
Br(1)–C(25)	1.904(5)	C(5)–C(6)	1.440(7)	C(13)–C(14)	1.402(8)
O(1)–C(22)	1.348(6)	C(6)–C(7)	1.399(7)	C(13)–C(17)	1.419(7)
N(1)–C(1)	1.279(7)	C(6)–C(16)	1.410(7)	C(14)–C(15)	1.376(7)
N(1)–C(2)	1.411(6)	C(7)–C(8)	1.388(8)	C(16)–C(17)	1.427(7)
C(1)–C(21)	1.452(7)	C(8)–C(9)	1.394(8)	C(21)–C(22)	1.407(7)
C(2)–C(3)	1.411(7)	C(9)–C(10)	1.400(7)	C(21)–C(26)	1.397(7)
C(2)–C(15)	1.392(7)	C(10)–C(11)	1.429(7)	C(22)–C(23)	1.385(7)
C(3)–C(4)	1.431(7)	C(10)–C(16)	1.423(6)	C(23)–C(24)	1.369(8)
C(3)–C(17)	1.417(7)	C(11)–C(12)	1.349(8)	C(24)–C(25)	1.404(7)
C(4)–C(5)	1.352(8)	C(12)–C(13)	1.434(7)	C(25)–C(26)	1.362(7)
Bond angles					
C(1)–N(1)–C(2)	120.8(5)	C(6)–C(16)–C(17)	120.1(4)	C(15)–C(2)–C(3)	120.5(4)
N(1)–C(1)–C(21)	121.9(5)	C(7)–C(6)–C(5)	121.7(5)	C(15)–C(14)–C(13)	120.4(4)
C(3)–C(2)–N(1)	118.2(4)	C(7)–C(6)–C(16)	119.6(5)	C(16)–C(6)–C(5)	118.7(5)
C(15)–C(2)–N(1)	121.1(5)	C(7)–C(8)–C(9)	120.4(5)	C(16)–C(10)–C(11)	119.1(5)
O(1)–C(22)–C(21)	121.2(4)	C(8)–C(7)–C(6)	120.5(5)	C(17)–C(3)–C(4)	118.4(5)
O(1)–C(22)–C(23)	118.8(5)	C(8)–C(9)–C(10)	120.8(5)	C(17)–C(13)–C(12)	119.3(5)
C(24)–C(25)–Br(1)	118.5(4)	C(9)–C(10)–C(11)	122.1(5)	C(22)–C(21)–C(1)	121.6(5)
C(26)–C(25)–Br(1)	120.7(4)	C(9)–C(10)–C(16)	118.7(5)	C(23)–C(22)–C(21)	120.0(5)
C(2)–C(3)–C(4)	123.3(4)	C(10)–C(16)–C(17)	119.9(5)	C(23)–C(24)–C(25)	119.3(5)
C(2)–C(3)–C(17)	118.2(4)	C(11)–C(12)–C(13)	121.4(5)	C(24)–C(23)–C(22)	120.8(5)
C(3)–C(17)–C(13)	120.6(5)	C(12)–C(11)–C(10)	121.0(5)	C(25)–C(26)–C(21)	120.5(5)
C(3)–C(17)–C(16)	120.1(5)	C(13)–C(17)–C(16)	119.3(4)	C(26)–C(21)–C(1)	119.7(5)
C(4)–C(5)–C(6)	121.1(5)	C(14)–C(13)–C(12)	121.6(5)	C(26)–C(21)–C(22)	118.7(5)
C(5)–C(4)–C(3)	121.6(5)	C(14)–C(13)–C(17)	119.1(5)	C(26)–C(25)–C(24)	120.8(5)
C(6)–C(16)–C(10)	120.0(5)	C(14)–C(15)–C(2)	121.1(5)		
Torsion angles					
C(1)–N(1)–C(2)–C(3)	149.5(5)	C(1)–N(1)–C(2)–C(15)	–34.2(9)		

Table S3 Selected bond lengths (Å) and bond angles (°) for **5**

Bond lengths					
Cl(1)–C(23)	1.729(2)	C(5)–C(6)	1.433(3)	C(13)–C(14)	1.400(3)
Cl(2)–C(25)	1.740(2)	C(6)–C(7)	1.400(3)	C(13)–C(17)	1.432(3)
O(1)–C(22)	1.337(3)	C(6)–C(16)	1.423(3)	C(14)–C(15)	1.375(3)
N(1)–C(1)	1.284(3)	C(7)–C(8)	1.389(4)	C(16)–C(17)	1.427(3)
N(1)–C(2)	1.412(3)	C(8)–C(9)	1.381(3)	C(21)–C(22)	1.417(3)
C(1)–C(21)	1.454(3)	C(9)–C(10)	1.403(3)	C(21)–C(26)	1.403(3)
C(2)–C(3)	1.412(3)	C(10)–C(11)	1.439(3)	C(22)–C(23)	1.393(3)
C(2)–C(15)	1.403(3)	C(10)–C(16)	1.416(3)	C(23)–C(24)	1.381(3)
C(3)–C(4)	1.434(3)	C(11)–C(12)	1.355(3)	C(24)–C(25)	1.392(3)
C(3)–C(17)	1.417(3)	C(12)–C(13)	1.423(3)	C(25)–C(26)	1.369(3)
C(4)–C(5)	1.353(3)				
Bond angles					
C(1)–N(1)–C(2)	121.82(18)	C(6)–C(16)–C(17)	119.5(2)	C(14)–C(15)–C(2)	120.8(2)
N(1)–C(1)–C(21)	120.99(19)	C(7)–C(6)–C(5)	123.0(2)	C(15)–C(2)–C(3)	119.7(2)
C(3)–C(2)–N(1)	117.38(17)	C(7)–C(6)–C(16)	118.8(2)	C(15)–C(14)–C(13)	121.81(18)
C(15)–C(2)–N(1)	122.71(19)	C(8)–C(7)–C(6)	120.9(2)	C(16)–C(6)–C(5)	118.3(2)
O(1)–C(22)–C(23)	120.18(19)	C(8)–C(9)–C(10)	120.9(2)	C(16)–C(10)–C(11)	119.2(2)
O(1)–C(22)–C(21)	121.7(2)	C(9)–C(8)–C(7)	120.4(2)	C(16)–C(17)–C(13)	118.9(2)
C(22)–C(23)–Cl(1)	119.26(17)	C(9)–C(10)–C(11)	121.9(2)	C(17)–C(3)–C(4)	118.3(2)
C(24)–C(23)–Cl(1)	118.63(17)	C(9)–C(10)–C(16)	119.0(2)	C(22)–C(21)–C(1)	120.8(2)
C(24)–C(25)–Cl(2)	118.75(18)	C(10)–C(16)–C(6)	120.0(2)	C(23)–C(22)–C(21)	118.1(2)
C(26)–C(25)–Cl(2)	120.15(17)	C(10)–C(16)–C(17)	120.51(18)	C(23)–C(24)–C(25)	118.9(2)
C(2)–C(3)–C(4)	122.5(2)	C(11)–C(12)–C(13)	122.30(19)	C(24)–C(23)–C(22)	122.09(19)
C(2)–C(3)–C(17)	119.17(18)	C(12)–C(11)–C(10)	120.2(2)	C(25)–C(26)–C(21)	120.25(19)
C(3)–C(17)–C(13)	120.5(2)	C(12)–C(13)–C(17)	119.0(2)	C(26)–C(21)–C(1)	119.59(19)
C(3)–C(17)–C(16)	120.65(18)	C(14)–C(13)–C(12)	123.06(18)	C(26)–C(21)–C(22)	119.6(2)
C(4)–C(5)–C(6)	122.05(19)	C(14)–C(13)–C(17)	118.0(2)	C(26)–C(25)–C(24)	121.1(2)
C(5)–C(4)–C(3)	121.0(2)				
Torsion angles					
C(1)–N(1)–C(2)–C(3)	160.6(2)	C(1)–N(1)–C(2)–C(15)	–24.6(3)		

Table S4 Selected bond lengths (Å) and bond angles (°) for **6**

Bond lengths					
Br(1)–C(23)	1.888(5)	C(5)–C(6)	1.439(6)	C(13)–C(14)	1.392(6)
Br(2)–C(25)	1.898(4)	C(6)–C(7)	1.401(6)	C(13)–C(17)	1.411(6)
O(1)–C(22)	1.324(5)	C(6)–C(16)	1.403(6)	C(14)–C(15)	1.384(7)
N(1)–C(1)	1.280(6)	C(7)–C(8)	1.382(7)	C(16)–C(17)	1.430(6)
N(1)–C(2)	1.413(6)	C(8)–C(9)	1.387(8)	C(21)–C(22)	1.415(6)
C(1)–C(21)	1.452(6)	C(9)–C(10)	1.400(7)	C(21)–C(26)	1.401(6)
C(2)–C(3)	1.415(6)	C(10)–C(11)	1.434(7)	C(22)–C(23)	1.399(7)
C(2)–C(15)	1.390(7)	C(10)–C(16)	1.426(6)	C(23)–C(24)	1.373(6)
C(3)–C(4)	1.427(6)	C(11)–C(12)	1.348(7)	C(24)–C(25)	1.383(7)
C(3)–C(17)	1.414(6)	C(12)–C(13)	1.434(7)	C(25)–C(26)	1.371(7)
C(4)–C(5)	1.353(6)				
Bond angles					
C(1)–N(1)–C(2)	121.2(4)	C(6)–C(16)–C(17)	120.6(4)	C(14)–C(15)–C(2)	121.0(4)
N(1)–C(1)–C(21)	121.6(5)	C(7)–C(6)–C(5)	122.1(5)	C(15)–C(2)–C(3)	120.0(4)
C(3)–C(2)–N(1)	117.5(4)	C(7)–C(6)–C(16)	119.4(4)	C(15)–C(14)–C(13)	121.0(5)
C(15)–C(2)–N(1)	122.4(4)	C(8)–C(7)–C(6)	120.8(5)	C(16)–C(6)–C(5)	118.5(4)
O(1)–C(22)–C(21)	121.7(5)	C(8)–C(9)–C(10)	121.0(5)	C(16)–C(10)–C(11)	119.5(4)
O(1)–C(22)–C(23)	120.4(5)	C(9)–C(8)–C(7)	120.2(4)	C(16)–C(17)–C(13)	119.7(4)
C(22)–C(23)–Br(1)	118.3(3)	C(9)–C(10)–C(11)	122.0(4)	C(17)–C(3)–C(4)	119.9(4)
C(24)–C(23)–Br(1)	119.8(4)	C(9)–C(10)–C(16)	118.6(5)	C(22)–C(21)–C(1)	121.1(4)
C(24)–C(25)–Br(2)	119.5(3)	C(10)–C(16)–C(6)	120.0(4)	C(23)–C(22)–C(21)	117.9(4)
C(26)–C(25)–Br(2)	119.3(4)	C(10)–C(16)–C(17)	119.4(4)	C(23)–C(24)–C(25)	119.3(4)
C(2)–C(3)–C(4)	121.9(4)	C(11)–C(12)–C(13)	121.6(5)	C(24)–C(23)–C(22)	121.9(4)
C(2)–C(3)–C(17)	118.2(4)	C(12)–C(11)–C(10)	120.6(4)	C(25)–C(26)–C(21)	120.1(4)
C(3)–C(17)–C(13)	121.3(4)	C(12)–C(13)–C(17)	119.3(4)	C(26)–C(21)–C(1)	119.1(4)
C(3)–C(17)–C(16)	118.9(4)	C(14)–C(13)–C(12)	122.3(4)	C(26)–C(21)–C(22)	119.7(4)
C(4)–C(5)–C(6)	121.5(4)	C(14)–C(13)–C(17)	118.4(4)	C(26)–C(25)–C(24)	121.1(4)
C(5)–C(4)–C(3)	120.5(4)				
Torsion angles					
C(1)–N(1)–C(2)–C(3)	155.9(4)	C(1)–N(1)–C(2)–C(15)	–28.2(6)		

Table S5 Selected bond lengths (Å) and bond angles (°) for **7**

Molecule A		Molecule B	
Bond lengths			
O(2)–C(27)	1.419(5)	O(2A)–C(27A)	1.421(5)
C(22)–O(1)	1.353(5)	C(22A)–O(1A)	1.353(5)
C(23)–O(2)	1.367(5)	C(23A)–O(2A)	1.376(5)
N(1)–C(1)	1.292(5)	N(1A)–C(1A)	1.290(5)
N(1)–C(2)	1.409(5)	N(1A)–C(2A)	1.412(5)
C(1)–C(21)	1.442(6)	C(1A)–C(21A)	1.445(6)
C(2)–C(3)	1.414(6)	C(2A)–C(3A)	1.401(6)
C(2)–C(15)	1.388(6)	C(2A)–C(15A)	1.388(6)
C(3)–C(4)	1.425(5)	C(3A)–C(4A)	1.446(5)
C(3)–C(17)	1.432(5)	C(3A)–C(17A)	1.416(5)
C(4)–C(5)	1.352(6)	C(4A)–C(5A)	1.349(6)
C(5)–C(6)	1.431(5)	C(5A)–C(6A)	1.433(6)
C(6)–C(7)	1.388(6)	C(6A)–C(7A)	1.385(6)
C(6)–C(16)	1.419(5)	C(6A)–C(16A)	1.421(5)
C(7)–C(8)	1.384(6)	C(7A)–C(8A)	1.380(7)
C(8)–C(9)	1.378(6)	C(8A)–C(9A)	1.386(6)
C(9)–C(10)	1.398(6)	C(9A)–C(10A)	1.401(6)
C(10)–C(11)	1.426(6)	C(10A)–C(11A)	1.422(6)
C(10)–C(16)	1.427(5)	C(10A)–C(16A)	1.426(6)
C(11)–C(12)	1.347(6)	C(11A)–C(12A)	1.352(6)
C(12)–C(13)	1.441(6)	C(12A)–C(13A)	1.425(6)
C(13)–C(14)	1.396(6)	C(13A)–C(14A)	1.393(6)
C(13)–C(17)	1.415(5)	C(13A)–C(17A)	1.415(5)
C(14)–C(15)	1.369(6)	C(14A)–C(15A)	1.371(6)
C(16)–C(17)	1.417(6)	C(16A)–C(17A)	1.421(6)
C(21)–C(22)	1.395(6)	C(21A)–C(22A)	1.400(6)
C(21)–C(26)	1.410(6)	C(21A)–C(26A)	1.412(6)
C(22)–C(23)	1.410(6)	C(22A)–C(23A)	1.387(6)
C(23)–C(24)	1.374(5)	C(23A)–C(24A)	1.380(6)
C(24)–C(25)	1.390(6)	C(24A)–C(25A)	1.394(6)
C(25)–C(26)	1.365(6)	C(25A)–C(26A)	1.348(6)
Bond angles			
C(1)–N(1)–C(2)	121.7(3)	C(1A)–N(1A)–C(2A)	120.7(4)
N(1)–C(1)–C(21)	122.4(4)	N(1A)–C(1A)–C(21A)	122.5(4)
C(3)–C(2)–N(1)	117.2(3)	C(3A)–C(2A)–N(1A)	118.0(4)
C(15)–C(2)–N(1)	123.0(4)	C(15A)–C(2A)–N(1A)	122.3(4)
O(1)–C(22)–C(21)	122.3(4)	O(1A)–C(22A)–C(21A)	121.7(4)
O(1)–C(22)–C(23)	117.7(3)	O(1A)–C(22A)–C(23A)	118.3(3)
O(2)–C(23)–C(22)	115.3(3)	O(2A)–C(23A)–C(22A)	115.2(3)
O(2)–C(23)–C(24)	125.3(4)	O(2A)–C(23A)–C(24A)	124.7(4)

C(23)–O(2)–C(27)	116.6(3)	C(23A)–O(2A)–C(27A)	116.1(3)
C(2)–C(3)–C(4)	123.6(4)	C(2A)–C(3A)–C(4A)	123.0(4)
C(2)–C(3)–C(17)	118.4(3)	C(2A)–C(3A)–C(17A)	119.0(3)
C(3)–C(17)–C(13)	120.2(3)	C(3A)–C(17A)–C(13A)	120.2(4)
C(3)–C(17)–C(16)	120.0(3)	C(3A)–C(17A)–C(16A)	120.1(3)
C(4)–C(5)–C(6)	121.3(4)	C(4A)–C(5A)–C(6A)	121.6(4)
C(5)–C(4)–C(3)	121.9(4)	C(5A)–C(4A)–C(3A)	121.4(4)
C(6)–C(16)–C(17)	120.3(3)	C(6A)–C(16A)–C(17A)	120.5(3)
C(7)–C(6)–C(5)	122.3(4)	C(7A)–C(6A)–C(5A)	122.7(4)
C(7)–C(6)–C(16)	119.2(4)	C(7A)–C(6A)–C(16A)	119.2(4)
C(8)–C(7)–C(6)	121.1(4)	C(8A)–C(7A)–C(6A)	121.8(4)
C(8)–C(9)–C(10)	120.6(4)	C(8A)–C(9A)–C(10A)	121.7(4)
C(9)–C(8)–C(7)	120.6(4)	C(9A)–C(8A)–C(7A)	119.4(4)
C(9)–C(10)–C(11)	122.4(4)	C(9A)–C(10A)–C(11A)	123.1(4)
C(9)–C(10)–C(16)	119.2(4)	C(9A)–C(10A)–C(16A)	118.3(4)
C(10)–C(16)–C(6)	119.3(4)	C(10A)–C(16A)–C(6A)	119.6(4)
C(10)–C(16)–C(17)	120.5(3)	C(10A)–C(16A)–C(17A)	119.9(3)
C(11)–C(12)–C(13)	121.7(4)	C(11A)–C(12A)–C(13A)	121.2(4)
C(12)–C(11)–C(10)	121.2(4)	C(12A)–C(11A)–C(10A)	121.4(4)
C(12)–C(13)–C(17)	118.4(4)	C(12A)–C(13A)–C(17A)	119.1(4)
C(14)–C(13)–C(12)	122.8(4)	C(14A)–C(13A)–C(12A)	121.9(4)
C(14)–C(13)–C(17)	118.8(4)	C(14A)–C(13A)–C(17A)	119.0(4)
C(14)–C(15)–C(2)	121.8(4)	C(14A)–C(15A)–C(2A)	121.8(4)
C(15)–C(2)–C(3)	119.7(4)	C(15A)–C(2A)–C(3A)	119.6(4)
C(15)–C(14)–C(13)	120.9(4)	C(15A)–C(14A)–C(13A)	120.3(4)
C(16)–C(6)–C(5)	118.5(4)	C(16A)–C(6A)–C(5A)	118.1(4)
C(16)–C(10)–C(11)	118.3(4)	C(16A)–C(10A)–C(11A)	118.5(4)
C(16)–C(17)–C(13)	119.8(3)	C(16A)–C(17A)–C(13A)	119.6(3)
C(17)–C(3)–C(4)	118.0(3)	C(17A)–C(3A)–C(4A)	118.1(4)
C(22)–C(21)–C(1)	121.3(4)	C(22A)–C(21A)–C(1A)	121.3(3)
C(23)–C(22)–C(21)	120.0(3)	C(23A)–C(22A)–C(21A)	120.0(4)
C(23)–C(24)–C(25)	120.9(4)	C(23A)–C(24A)–C(25A)	119.9(4)
C(24)–C(23)–C(22)	119.4(4)	C(24A)–C(23A)–C(22A)	120.1(4)
C(25)–C(26)–C(21)	120.8(4)	C(25A)–C(26A)–C(21A)	120.6(4)
C(26)–C(21)–C(1)	119.8(4)	C(26A)–C(21A)–C(1A)	120.0(4)
C(26)–C(21)–C(22)	118.8(4)	C(26A)–C(21A)–C(22A)	118.7(4)
C(26)–C(25)–C(24)	120.0(4)	C(26A)–C(25A)–C(24A)	120.7(4)
Torsion angles			
C(1)–N(1)–C(2)–C(3)	–158.2(4)	C(1A)–N(1A)–C(2A)–C(3A)	156.0(4)
C(1)–N(1)–C(2)–C(15)	25.6(6)	C(1A)–N(1A)–C(2A)–C(15A)	–28.3(6)

Table S6. Hydrogen bond lengths (Å) and angles (°) for **2**, **3** and **5–7**

	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠(DHA)
2		0.96(5)	1.74(5)	2.594(3)	147(4)
3		1.07(14)	1.63(13)	2.604(6)	148(11)
5	O(1)–H(1O)···N(1)	0.84(4)	1.77(3)	2.577(2)	159(3)
6		0.96(7)	1.78(7)	2.600(6)	141(5)
		0.84	1.79	2.612(4)	167.0
7	O(1A)–H(1OA)···N(1A)	0.84	1.90	2.607(5)	141.7

Table S7. π···π bond lengths (Å) and angles (°) for **2**, **3** and **5–7**[a]

	Cg(*I*)	Cg(*J*)[b]	*d*[Cg(*I*)–Cg(*J*)]	*α*	*β*
2[b]	Cg(1)	Cg(2)$^{\#1}$	3.617(2)	0.17	20.43
	Cg(1)	Cg(3)$^{\#1}$	4.1215(18)	0.47	34.36
	Cg(1)	Cg(4)$^{\#1}$	3.612(2)	0.39	19.94
	Cg(2)	Cg(1)$^{\#2}$	3.617(2)	0.17	20.29
	Cg(2)	Cg(3)$^{\#1}$	3.621(2)	0.59	20.07
	Cg(2)	Cg(4)$^{\#1}$	4.598(2)	0.44	42.57
	Cg(2)	Cg(4)$^{\#2}$	4.601(2)	0.44	42.63
	Cg(3)	Cg(1)$^{\#2}$	4.1217(18)	0.47	34.83
	Cg(3)	Cg(2)$^{\#2}$	3.621(2)	0.59	20.09
	Cg(3)	Cg(4)$^{\#2}$	3.622(2)	0.26	20.34
	Cg(4)	Cg(1)$^{\#2}$	3.612(2)	0.39	20.23
	Cg(4)	Cg(2)$^{\#1}$	4.601(2)	0.44	42.27
	Cg(4)	Cg(2)$^{\#2}$	4.598(2)	0.44	42.41
	Cg(4)	Cg(3)$^{\#1}$	3.622(2)	0.26	20.11
3[b]	Cg(1)	Cg(2)$^{\#2}$	3.631(3)	0.19	20.38
	Cg(1)	Cg(3)$^{\#2}$	4.102(3)	0.47	33.49
	Cg(1)	Cg(4)$^{\#2}$	3.617(3)	0.56	19.53
	Cg(2)	Cg(1)$^{\#1}$	3.631(3)	0.19	20.21
	Cg(2)	Cg(3)$^{\#2}$	3.630(3)	0.36	19.81
	Cg(2)	Cg(4)$^{\#1}$	4.643(3)	0.46	42.82
	Cg(2)	Cg(4)$^{\#2}$	4.628(3)	0.46	42.7
	Cg(3)	Cg(1)$^{\#1}$	4.102(3)	0.47	33.9
	Cg(3)	Cg(2)$^{\#1}$	3.629(3)	0.36	19.89
	Cg(3)	Cg(4)$^{\#1}$	3.636(3)	0.10	20.01
	Cg(4)	Cg(1)$^{\#1}$	3.617(3)	0.56	19.83
	Cg(4)	Cg(2)$^{\#1}$	4.627(3)	0.46	42.46
	Cg(4)	Cg(2)$^{\#2}$	4.642(3)	0.46	42.49
	Cg(4)	Cg(3)$^{\#2}$	3.636(3)	0.10	20
5[b]	Cg(1)	Cg(1)$^{\#3}$	4.3405(16)	0.00	36.87
	Cg(1)	Cg(1)$^{\#4}$	4.6370(16)	0.00	43.97
	Cg(1)	Cg(2)$^{\#3}$	3.8427(16)	3.38	23.93
	Cg(1)	Cg(2)$^{\#4}$	4.8675(17)	3.38	47.36
	Cg(1)	Cg(3)$^{\#3}$	3.7798(15)	3.98	26.18
	Cg(1)	Cg(4)$^{\#3}$	3.5778(15)	2.65	17.54
	Cg(2)	Cg(1)$^{\#3}$	3.8428(16)	3.38	27.17
	Cg(2)	Cg(1)$^{\#4}$	4.8674(17)	3.38	49.19
	Cg(2)	Cg(2)$^{\#3}$	4.7646(16)	0.00	44.69
	Cg(2)	Cg(4)$^{\#3}$	3.8347(15)	2.57	26.52
	Cg(3)	Cg(1)$^{\#3}$	3.7799(15)	3.98	24.8
	Cg(3)	Cg(5)$^{\#4}$	4.4971(16)	30.26	27.89
	Cg(4)	Cg(1)$^{\#3}$	3.5778(15)	2.65	17.03
	Cg(4)	Cg(2)$^{\#3}$	3.8347(15)	2.57	24.2

	Cg(4)	Cg(4)$^{\#3}$	4.3353(15)	0.00	36.8
	Cg(4)	Cg(5)$^{\#4}$	4.0737(15)	28.87	14.3
	Cg(5)	Cg(3)$^{\#4}$	4.4971(16)	30.26	57.7
	Cg(5)	Cg(4)$^{\#4}$	4.0737(15)	28.87	33.6
	Cg(5)	Cg(5)$^{\#3}$	3.8615(15)	0.00	27.48
6[b]	Cg(1)	Cg(2)$^{\#5}$	3.712(2)	0.54	23.61
	Cg(1)	Cg(3)$^{\#5}$	4.055(2)	1.71	31.81
	Cg(1)	Cg(4)$^{\#5}$	3.544(2)	0.38	15.88
	Cg(2)	Cg(1)$^{\#6}$	3.712(2)	0.54	23.15
	Cg(2)	Cg(3)$^{\#5}$	3.582(2)	1.53	16.22
	Cg(2)	Cg(4)$^{\#6}$	4.831(3)	0.41	44.79
	Cg(2)	Cg(4)$^{\#5}$	4.569(3)	0.41	41.86
	Cg(3)	Cg(1)$^{\#6}$	4.055(2)	1.71	33.52
	Cg(3)	Cg(2)$^{\#6}$	3.582(2)	1.53	15.72
	Cg(3)	Cg(4)$^{\#6}$	3.747(3)	1.35	23.54
	Cg(4)	Cg(1)$^{\#6}$	3.544(2)	0.38	15.95
	Cg(4)	Cg(2)$^{\#6}$	4.570(3)	0.41	41.52
	Cg(4)	Cg(2)$^{\#5}$	4.831(3)	0.41	45.06
	Cg(4)	Cg(3)$^{\#5}$	3.747(3)	1.35	23.27
7[c]	Cg(1)	Cg(1)$^{\#1}$	3.679(2)	0.00	21.35
	Cg(1)	Cg(3)$^{\#1}$	3.707(2)	2.79	22.23
	Cg(1)	Cg(7)$^{\#1}$	4.446(2)	3.52	38.1
	Cg(1)	Cg(9)$^{\#2}$	4.122(2)	25.86	39.67
	Cg(2)	Cg(2)$^{\#3}$	3.698(2)	0.00	18.87
	Cg(2)	Cg(4)$^{\#3}$	3.858(2)	2.85	25.23
	Cg(2)	Cg(8)$^{\#3}$	4.549(2)	3.04	38.54
	Cg(2)	Cg(10)$^{\#4}$	4.089(2)	29.08	35.04
	Cg(3)	Cg(1)$^{\#1}$	3.707(2)	2.79	23.86
	Cg(3)	Cg(5)$^{\#5}$	4.409(2)	46.31	10.41
	Cg(4)	Cg(2)$^{\#3}$	3.858(2)	2.85	26.31
	Cg(4)	Cg(6)$^{\#6}$	4.389(2)	40.79	12.65
	Cg(5)	Cg(3)$^{\#6}$	4.409(2)	46.31	56.71
	Cg(5)	Cg(5)$^{\#5}$	4.913(2)	45.76	27.57
	Cg(5)	Cg(5)$^{\#6}$	4.913(2)	45.76	54.39
	Cg(6)	Cg(4)$^{\#5}$	4.389(2)	40.79	53.39
	Cg(6)	Cg(6)$^{\#5}$	4.912(2)	39.75	52.41
	Cg(6)	Cg(6)$^{\#6}$	4.912(2)	39.75	28.84
	Cg(7)	Cg(1)$^{\#1}$	4.446(2)	3.52	40.63
	Cg(7)	Cg(9)$^{\#4}$	4.497(2)	25.06	43.61
	Cg(8)	Cg(2)$^{\#3}$	4.549(2)	3.04	40.78
	Cg(8)	Cg(10)$^{\#4}$	4.569(2)	27.87	41.31
	Cg(9)	Cg(1)$^{\#2}$	4.122(2)	25.86	14.95
	Cg(9)	Cg(7)$^{\#2}$	4.497(2)	25.06	29.18
	Cg(10)	Cg(2)$^{\#4}$	4.089(2)	29.08	9.5

Cg(10)	Cg(8)[#4]	4.569(2)	27.87	25.43

[a] Cg(*I*)–Cg(*J*): distance between ring centroids; α: dihedral angle between planes Cg(*I*) and Cg(*J*); β: angle Cg(*I*) → Cg(*J*) vector and normal to plane *I*.

[b] Symmetry transformations used to generate equivalent atoms: #1 –1 + *x*, *y*, *z*; #2 1 + *x*, *y*, *z*; #3 1 – *x*, –*y*, 1 – *z*; #4 1 – *x*, 1 – *y*, 1 – *z*; #5 *x*, 1 + *y*, *z*; #6 *x*, –1 + *y*, *z*; #7 1 – *x*, 1 – *y*, 2 – *z*; #8 2 – *x*, 1 – *y*, 1 – *z*; #9 2 – *x*, 1 – *y*, 2 – *z*; #10 *x*, 1/2 – *y*, –1/2 + *z*; #11 *x*, 1/2 – *y*, 1/2 + *z*. Cg(1): C(2)–C(3)–C(17)–C(13)–C(14)–C(15), Cg(2): C(3)–C(4)–C(5)–C(6)–C(16)–C(17), Cg(3): C(6)–C(7)–C(8)–C(9)–C(10)–C(16), Cg(4): C(10)–C(11)–C(12)–C(13)–C(17)–C(16), Cg(5): C(21)–C(22)–C(23)–C(24)–C(25)–C(26).

[c] Symmetry transformations used to generate equivalent atoms: #1 1 – *x*, 1 – *y*, 2 – *z*; #2 1 – *x*, 1 – *y*, 1 – *z*; #3 2 – *x*, 1 – *y*, 1 – *z*; #4 2 – *x*, 1 – *y*, 2 – *z*; #5 *x*, 1/2 – *y*, –1/2 + *z*; #6 *x*, 1/2 – *y*, 1/2 + *z*. Cg(1): C(2)–C(3)–C(17)–C(13)–C(14)–C(15), Cg(2): C(2A)–C(3A)–C(17A)–C(13A)–C(14A)–C(15A), Cg(3): C(3)–C(4)–C(5)–C(6)–C(16)–C(17), Cg(4): C(3A)–C(4A)–C(5A)–C(6A)–C(16A)–C(17A), Cg(5): C(6)–C(7)–C(8)–C(9)–C(10)–C(16), Cg(6): C(6A)–C(7A)–C(8A)–C(9A)–C(10A)–C(16A), Cg(7): C(10)–C(11)–C(12)–C(13)–C(17)–C(16), Cg(8): C(10A)–C(11A)–C(12A)–C(13A)–C(17A)–C(16A), Cg(9): C(21)–C(22)–C(23)–C(24)–C(25)–C(26), Cg(10): C(21A)–C(22A)–C(23A)–C(24A)–C(25A)–C(26A).