An investigation on single crystal growth, structural, thermal and optical properties of a series of organic D $-\pi$ –A push-pull materials

Vinod Kumar Gupta and Ram Adhar Singh*

Department of Chemistry, Centre of Advanced Study, Faculty of Science, Banaras Hindu University, Varanasi-221 005, INDIA

Email: prrasingh@gmail.com

Supporting Information

I.	NMR spectra (¹ H and ¹³ C)	Figs. S1 to S8
II.	Solubility in 1:2 acetone-methanol mixture	Table S1
III.	Plots of 1/T versus lnN _s	Fig. S9
IV.	Crystal structure study and refinement	
V	Bond lengths and bond angles	Table S2
VI.	View of C–H π interactions	Figs. S10 to S12
VII	Orientation of molecules in unit cell	Figs. S13
VIII.	Thermal activation energy plots	Figs. S14
IX.	UV-Visible absorption spectra in different solvents	Figs. S15
X.	Fluorescence spectra in different solvents	Figs. S16
XI.	Lippert-Mataga plots	Figs. S17

I. NMR spectra (¹H and ¹³C)



Fig. S1: ¹H NMR spectrum of chromophore 1



Fig. S2: ¹³C NMR spectrum of chromophore 1



Fig. S3: ¹H NMR spectrum of chromophore 2



Fig. S4: ¹³C NMR spectrum of chromophore 2



Fig. S5: ¹H NMR spectrum of chromophore 3



Fig. S6: ¹³C NMR spectrum of chromophore 3



Fig. S7: ¹H NMR spectrum of chromophore 4



Fig. S8: ¹³C NMR spectrum of chromophore 4

Chromophore	Solubility (g/100 g of solvent)ª
1	0.49
2	0.61
3	2.60
4	1.10

II. Table S1: Solubility in 1:2 acetone-methanol mixture

^aSolubility at 28.0 °C in mixed 1:2 acetone-methanol (by weight) solvent.

III. Plots of 1/T versus lnN_s



Fig. S9: Plot of 1/T versus $\ln N_s$ for (a) chromophore 1, (b) chromophore 2, (c) chromophore 3 and (d) chromophore 4 in 1:1 acetone-methanol mixed solvent.

IV. Crystal structure study and refinement

For single crystal X-ray diffraction studies, a suitable single crystal of all the chromophores with approximate dimensions were selected and mounted on a glass needle with the help of grease. The crystal's diffractions were recorded by using the Xcalibur oxford CCD diffractometer. The data reduction was carried out using Chrysalis Pro software. The structures were solved by direct method (SHELXL-97) and refined against all data by full matrix least-square on F^2 using anisotropic displacement parameters for all non-hydrogen

atoms. All hydrogen atoms were included in the refinement at geometrically ideal positions and refined with a riding model.

V. Bond lengths and bond angles

 Table S2: Bond Lengths (Å) and Bond Angles (deg) in the Structures Studied

Chromophore 1							
N(2)–C(6)	1.359(4)	N(2)–C(10)	1.450(4)	N(2)–C(9)	1.453(4)		
C(6)-C(7)	1.407(4)	C(6) - C(5)	1.415(4)	C(3)-C(4)	1.375(4)		
C(3) - C(8)	1.388(5)	C(3) - C(2)	1.503(6)	C(8) - C(7)	1.389(5)		
C(8)–H(8)	0.9300	C(5) - C(4)	1.363(4)	C(5)–H(5)	0.9300		
C(7)–H(7)	0.9300	C(4)–H(4)	0.9300	C(10)–H(10A)	0.9600		
C(10)–H(10B)	0.9600	C(10)–H(10C)	0.9600	C(2)-C(1)	1.238(6)		
C(2)-H(2)	0.9300	C(9)–H(9A)	0.9600	C(9)–H(9B)	0.9600		
C(9)-H(9C)	0.9600	O(2) - N(1)	1.238(5)	N(1) - O(1)	1.220(5)		
N(1) - C(1)	1.443(5)	C(1) - H(1)	0.9300				
C(6)-N(2)-C(10)	121.4(3)	C(6)-N2-C(9)	120.9(3)	C(10)-N(2)-C(9)	117.1(3)		
N(2)-C(6)-C(7)	123.1(3)	N(2)-C(6)-C(5)	121.1(3)	C(7)-C(6)-C(5)	115.8(3)		
C(4)-C(3)-C(8)	116.3(3)	C(4)-C(3)-C(2)	117.5(3)	C(8)-C(3)-C(2)	126.2(3)		
C(3)–C(8)–C(7)	122.3(3)	C(3)–C(8)–H(8)	118.8	C(7)–C(8)–H(8)	118.8		
C(4)-C(5)-C(6)	121.4(3)	C(4)-C(5)-H(5)	119.3	C(6)-C(5)-H(5)	119.3		
C(8)-C(7)-C(6)	120.9(3)	C(8)–C(7)–H(7)	119.6	C(6)–C(7)–H(7)	119.6		
C(5)-C(4)-C(3)	123.2(3)	C(5)-C(4)-H(4)	118.4	C(3)-C(4)-H(4)	118.4		
N(2)–C(10)–H(10A)	109.5	N(2)-C(10)-H(10B)	109.5	H(10A)-C(10)-H(10B)	109.5		
N(2)–C(10)–H(10C)	109.5	H(10A)–C(10)–H(10C)	109.5	H(10B)-C(10)-H(10C)	109.5		
C(1)-C(2)-C(3)	126.7(5)	C(1)-C(2)-H(2)	116.7	C(3)-C(2)-H(2)	116.7		
N(2)-C(9)-H(9A)	109.5	N(2)-C(9)-H(9B)	109.5	H9(A)–C(9)–H(9B)	109.5		
N(2)-C(9)-H(9C)	109.5	H(9A)–C(9)–H(9C)	109.5	H(9B)-C(9)-H(9C)	109.5		
O(1) - N(1) - O(2)	122.6(4)	O(1) - N(1) - C(1)	113.1(5)	O(2)-N(1)-C(1)	124.3(4)		
C(2)-C(1)-N(1)	120.6(5	C(2) - C(1) - H(1)	119.7	N(1) - C(1) - H(1)	119.7		
		Chromophore 2					
N(1)-C(1)	1.352(4)	Chromophore 2 N(1)–C(11)	1.453(4)	N(1)-C(12)	1.455(4)		
N(1)-C(1) C(2)-C(3)	1.352(4) 1.375(4)	Chromophore 2 N(1)–C(11) C(2)–C(1)	1.453(4) 1.395(4)	N(1)–C(12) C(2)–H(2)	1.455(4) 0.9300		
N(1)-C(1) C(2)-C(3) C(4)-C(3)	1.352(4) 1.375(4) 1.386(4)	Chromophore 2 N(1)–C(11) C(2)–C(1) C(4)–C(5)	1.453(4) 1.395(4) 1.415(4)	N(1)-C(12) C(2)-H(2) C(4)-C(7)	1.455(4) 0.9300 1.422(4)		
N(1)-C(1) C(2)-C(3) C(4)-C(3) C(1)-C(6)	1.352(4) 1.375(4) 1.386(4) 1.406(4)	Chromophore 2 N(1)–C(11) C(2)–C(1) C(4)–C(5) C(6)–C(5)	1.453(4) 1.395(4) 1.415(4) 1.373(3)	N(1)-C(12) C(2)-H(2) C(4)-C(7) C(6)-H(6)	1.455(4) 0.9300 1.422(4) 0.9300		
N(1)-C(1) C(2)-C(3) C(4)-C(3) C(1)-C(6) C(5)-H(5)	1.352(4) 1.375(4) 1.386(4) 1.406(4) 0.9300	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3)	1.453(4) 1.395(4) 1.415(4) 1.373(3) 0.9300	N(1)-C(12) C(2)-H(2) C(4)-C(7) C(6)-H(6) C(8)-C(7)	1.455(4) 0.9300 1.422(4) 0.9300 1.367(4)		
N(1)-C(1) C(2)-C(3) C(4)-C(3) C(1)-C(6) C(5)-H(5) C(8)-C(9)	1.352(4) 1.375(4) 1.386(4) 1.406(4) 0.9300 1.417(4)	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10)	1.453(4) 1.395(4) 1.415(4) 1.373(3) 0.9300 1.430(4)	N(1)-C(12) C(2)-H(2) C(4)-C(7) C(6)-H(6) C(8)-C(7) C(7)-H(7)	1.455(4) 0.9300 1.422(4) 0.9300 1.367(4) 0.9300		
N(1)-C(1) C(2)-C(3) C(4)-C(3) C(1)-C(6) C(5)-H(5) C(8)-C(9) C(11)-H(11B)	1.352(4) 1.375(4) 1.386(4) 1.406(4) 0.9300 1.417(4) 0.9600	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C)	1.453(4) 1.395(4) 1.415(4) 1.373(3) 0.9300 1.430(4) 0.9600	N(1)-C(12) C(2)-H(2) C(4)-C(7) C(6)-H(6) C(8)-C(7) C(7)-H(7) C(11)-H(11A)	1.455(4) 0.9300 1.422(4) 0.9300 1.367(4) 0.9300 0.9600		
N(1)-C(1) C(2)-C(3) C(4)-C(3) C(1)-C(6) C(5)-H(5) C(8)-C(9) C(11)-H(11B) C(12)-H(12B)	$\begin{array}{c} 1.352(4) \\ 1.375(4) \\ 1.386(4) \\ 1.406(4) \\ 0.9300 \\ 1.417(4) \\ 0.9600 \\ 0.9600 \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C)	$\begin{array}{c} 1.453(4) \\ 1.395(4) \\ 1.415(4) \\ 1.373(3) \\ 0.9300 \\ 1.430(4) \\ 0.9600 \\ 0.9600 \end{array}$	N(1)-C(12) C(2)-H(2) C(4)-C(7) C(6)-H(6) C(8)-C(7) C(7)-H(7) C(11)-H(11A) C(12)-H(12A)	1.455(4) 0.9300 1.422(4) 0.9300 1.367(4) 0.9300 0.9600 0.9600		
N(1)-C(1) C(2)-C(3) C(4)-C(3) C(1)-C(6) C(5)-H(5) C(8)-C(9) C(11)-H(11B) C(12)-H(12B) N(3)-C(9)	$\begin{array}{c} 1.352(4) \\ 1.375(4) \\ 1.386(4) \\ 1.406(4) \\ 0.9300 \\ 1.417(4) \\ 0.9600 \\ 0.9600 \\ 1.143(4) \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2)	$\begin{array}{c} 1.453(4) \\ 1.395(4) \\ 1.415(4) \\ 1.373(3) \\ 0.9300 \\ 1.430(4) \\ 0.9600 \\ 0.9600 \\ 1.127(4) \end{array}$	N(1)-C(12) C(2)-H(2) C(4)-C(7) C(6)-H(6) C(8)-C(7) C(7)-H(7) C(11)-H(11A) C(12)-H(12A)	$\begin{array}{c} 1.455(4) \\ 0.9300 \\ 1.422(4) \\ 0.9300 \\ 1.367(4) \\ 0.9300 \\ 0.9600 \\ 0.9600 \end{array}$		
$\begin{array}{c} N(1)-C(1) \\ C(2)-C(3) \\ C(4)-C(3) \\ C(1)-C(6) \\ C(5)-H(5) \\ C(8)-C(9) \\ C(11)-H(11B) \\ C(12)-H(12B) \\ N(3)-C(9) \end{array}$	$\begin{array}{c} 1.352(4) \\ 1.375(4) \\ 1.386(4) \\ 1.406(4) \\ 0.9300 \\ 1.417(4) \\ 0.9600 \\ 0.9600 \\ 1.143(4) \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2)	$1.453(4) \\ 1.395(4) \\ 1.415(4) \\ 1.373(3) \\ 0.9300 \\ 1.430(4) \\ 0.9600 \\ 0.9600 \\ 1.127(4) $	N(1)-C(12) $C(2)-H(2)$ $C(4)-C(7)$ $C(6)-H(6)$ $C(8)-C(7)$ $C(7)-H(7)$ $C(11)-H(11A)$ $C(12)-H(12A)$	1.455(4) 0.9300 1.422(4) 0.9300 1.367(4) 0.9300 0.9600 0.9600		
$\begin{array}{c} N(1)-C(1) \\ C(2)-C(3) \\ C(4)-C(3) \\ C(1)-C(6) \\ C(5)-H(5) \\ C(8)-C(9) \\ C(11)-H(11B) \\ C(12)-H(12B) \\ N(3)-C(9) \\ \end{array}$	$\begin{array}{c} 1.352(4) \\ 1.375(4) \\ 1.386(4) \\ 1.406(4) \\ 0.9300 \\ 1.417(4) \\ 0.9600 \\ 0.9600 \\ 1.143(4) \\ 122.3(3) \\ 122.1(4) \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12)	$1.453(4) \\ 1.395(4) \\ 1.415(4) \\ 1.373(3) \\ 0.9300 \\ 1.430(4) \\ 0.9600 \\ 0.9600 \\ 1.127(4) \\ 121.3(3) \\ 1420.2 \\ 1420.$	N(1)-C(12) $C(2)-H(2)$ $C(4)-C(7)$ $C(6)-H(6)$ $C(8)-C(7)$ $C(7)-H(7)$ $C(11)-H(11A)$ $C(12)-H(12A)$ $C(11)-N(1)-C(12)$	$\begin{array}{c} 1.455(4) \\ 0.9300 \\ 1.422(4) \\ 0.9300 \\ 1.367(4) \\ 0.9300 \\ 0.9600 \\ 0.9600 \\ \end{array}$		
$\begin{array}{c} N(1)-C(1) \\ C(2)-C(3) \\ C(4)-C(3) \\ C(1)-C(6) \\ C(5)-H(5) \\ C(8)-C(9) \\ C(11)-H(11B) \\ C(12)-H(12B) \\ N(3)-C(9) \\ \end{array}$	$\begin{array}{c} 1.352(4) \\ 1.375(4) \\ 1.386(4) \\ 1.406(4) \\ 0.9300 \\ 1.417(4) \\ 0.9600 \\ 0.9600 \\ 1.143(4) \\ 122.3(3) \\ 120.4(4) \\ 122.3(3) \\ 120.4(4) \\ 122.3(3) \\ 120.4(4) \\$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2)	1.453(4) 1.395(4) 1.415(4) 1.373(3) 0.9300 1.430(4) 0.9600 0.9600 1.127(4) 121.3(3) 119.8 119.8	N(1)-C(12) $C(2)-H(2)$ $C(4)-C(7)$ $C(6)-H(6)$ $C(8)-C(7)$ $C(7)-H(7)$ $C(11)-H(11A)$ $C(12)-H(12A)$ $C(11)-N(1)-C(12)$ $C(1)-C(2)-H(2)$	1.455(4) 0.9300 1.422(4) 0.9300 1.367(4) 0.9300 0.9600 0.9600 116.4(3) 119.8		
$\begin{array}{c} N(1)-C(1) \\ C(2)-C(3) \\ C(4)-C(3) \\ C(1)-C(6) \\ C(5)-H(5) \\ C(8)-C(9) \\ C(11)-H(11B) \\ C(12)-H(12B) \\ N(3)-C(9) \\ \end{array}$	$\begin{array}{c} 1.352(4) \\ 1.375(4) \\ 1.386(4) \\ 1.406(4) \\ 0.9300 \\ 1.417(4) \\ 0.9600 \\ 0.9600 \\ 1.143(4) \\ 122.3(3) \\ 120.4(4) \\ 116.4(4) \\ 116.4(4) \\$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(4)-C(7)	$\begin{array}{c} 1.453(4) \\ 1.395(4) \\ 1.415(4) \\ 1.373(3) \\ 0.9300 \\ 1.430(4) \\ 0.9600 \\ 0.9600 \\ 1.127(4) \\ 121.3(3) \\ 119.8 \\ 118.7(3) \\ 121.(2) \end{array}$	N(1)-C(12) $C(2)-H(2)$ $C(4)-C(7)$ $C(6)-H(6)$ $C(8)-C(7)$ $C(7)-H(7)$ $C(11)-H(11A)$ $C(12)-H(12A)$ $C(11)-N(1)-C(12)$ $C(1)-C(2)-H(2)$ $C(5)-C(4)-C(7)$	$1.455(4) \\ 0.9300 \\ 1.422(4) \\ 0.9300 \\ 1.367(4) \\ 0.9300 \\ 0.9600 \\ 0.9600 \\ 116.4(3) \\ 119.8 \\ 125.0(3) \\ 115.0(2) \\ 0.9600 \\$		
$\begin{array}{c} N(1)-C(1) \\ C(2)-C(3) \\ C(4)-C(3) \\ C(1)-C(6) \\ C(5)-H(5) \\ C(8)-C(9) \\ C(11)-H(11B) \\ C(12)-H(12B) \\ N(3)-C(9) \\ \hline \\ C(1)-N(1)-C(11) \\ C(3)-C(2)-C(1) \\ C(3)-C(4)-C(5) \\ N(1)-C(1)-C(2) \\ \hline \end{array}$	$\begin{array}{c} 1.352(4) \\ 1.375(4) \\ 1.386(4) \\ 1.406(4) \\ 0.9300 \\ 1.417(4) \\ 0.9600 \\ 0.9600 \\ 1.143(4) \\ 122.3(3) \\ 120.4(4) \\ 116.3(3) \\ 121.2(3) \\ \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6)	$\begin{array}{c} 1.453(4) \\ 1.395(4) \\ 1.415(4) \\ 1.373(3) \\ 0.9300 \\ 1.430(4) \\ 0.9600 \\ 0.9600 \\ 1.127(4) \\ 121.3(3) \\ 119.8 \\ 118.7(3) \\ 121.1(3) \\ 121.1(3) \end{array}$	N(1)-C(12) $C(2)-H(2)$ $C(4)-C(7)$ $C(6)-H(6)$ $C(8)-C(7)$ $C(7)-H(7)$ $C(11)-H(11A)$ $C(12)-H(12A)$ $C(11)-N(1)-C(12)$ $C(1)-C(2)-H(2)$ $C(5)-C(4)-C(7)$ $C(2)-C(1)-C(6)$	$\begin{array}{c} 1.455(4) \\ 0.9300 \\ 1.422(4) \\ 0.9300 \\ 1.367(4) \\ 0.9300 \\ 0.9600 \\ 0.9600 \\ \end{array}$ $\begin{array}{c} 116.4(3) \\ 119.8 \\ 125.0(3) \\ 117.6(3) \\ \end{array}$		
$\begin{array}{c} N(1)-C(1) \\ C(2)-C(3) \\ C(4)-C(3) \\ C(1)-C(6) \\ C(5)-H(5) \\ C(8)-C(9) \\ C(11)-H(11B) \\ C(12)-H(12B) \\ N(3)-C(9) \\ \hline \\ C(1)-N(1)-C(11) \\ C(3)-C(2)-C(1) \\ C(3)-C(4)-C(5) \\ N(1)-C(1)-C(2) \\ C(5)-C(6)-C(1) \\ \hline \end{array}$	$\begin{array}{c} 1.352(4) \\ 1.375(4) \\ 1.386(4) \\ 1.406(4) \\ 0.9300 \\ 1.417(4) \\ 0.9600 \\ 0.9600 \\ 1.143(4) \\ 122.3(3) \\ 120.4(4) \\ 116.3(3) \\ 121.2(3) \\$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6) C(5)-C(6)-H(6)	$\begin{array}{c} 1.453(4) \\ 1.395(4) \\ 1.415(4) \\ 1.373(3) \\ 0.9300 \\ 1.430(4) \\ 0.9600 \\ 0.9600 \\ 1.127(4) \\ 121.3(3) \\ 119.8 \\ 118.7(3) \\ 121.1(3) \\ 119.4 \\ \end{array}$	N(1)-C(12) $C(2)-H(2)$ $C(4)-C(7)$ $C(6)-H(6)$ $C(8)-C(7)$ $C(7)-H(7)$ $C(11)-H(11A)$ $C(12)-H(12A)$ $C(1)-C(2)-H(2)$ $C(5)-C(4)-C(7)$ $C(2)-C(1)-C(6)$ $C(1)-C(6)-H(6)$	$\begin{array}{c} 1.455(4) \\ 0.9300 \\ 1.422(4) \\ 0.9300 \\ 1.367(4) \\ 0.9300 \\ 0.9600 \\ 0.9600 \\ \end{array}$ $\begin{array}{c} 116.4(3) \\ 119.8 \\ 125.0(3) \\ 117.6(3) \\ 119.4 \\ \end{array}$		
$\begin{array}{c} N(1)-C(1)\\ C(2)-C(3)\\ C(4)-C(3)\\ C(1)-C(6)\\ C(5)-H(5)\\ C(8)-C(9)\\ C(11)-H(11B)\\ C(12)-H(12B)\\ N(3)-C(9)\\ \end{array}$	$\begin{array}{c} 1.352(4)\\ 1.375(4)\\ 1.386(4)\\ 1.406(4)\\ 0.9300\\ 1.417(4)\\ 0.9600\\ 0.9600\\ 1.143(4)\\ 122.3(3)\\ 120.4(4)\\ 116.3(3)\\ 121.2(3)\\ 121.2(3)\\ 121.4(3)\\ \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6) C(5)-C(6)-H(6) C(6)-C(5)-H(5)	$\begin{array}{c} 1.453(4)\\ 1.395(4)\\ 1.415(4)\\ 1.373(3)\\ 0.9300\\ 1.430(4)\\ 0.9600\\ 0.9600\\ 1.127(4)\\ 121.3(3)\\ 119.8\\ 118.7(3)\\ 121.1(3)\\ 119.4\\ 119.3\\ \end{array}$	$\begin{array}{c} N(1)-C(12)\\ C(2)-H(2)\\ C(4)-C(7)\\ C(6)-H(6)\\ C(8)-C(7)\\ C(7)-H(7)\\ C(11)-H(11A)\\ C(12)-H(12A)\\ \end{array}$	$\begin{array}{c} 1.455(4) \\ 0.9300 \\ 1.422(4) \\ 0.9300 \\ 1.367(4) \\ 0.9300 \\ 0.9600 \\ 0.9600 \\ \end{array}$ $\begin{array}{c} 116.4(3) \\ 119.8 \\ 125.0(3) \\ 117.6(3) \\ 119.4 \\ 119.3 \end{array}$		
$\begin{array}{c} N(1)-C(1) \\ C(2)-C(3) \\ C(4)-C(3) \\ C(1)-C(6) \\ C(5)-H(5) \\ C(8)-C(9) \\ C(11)-H(11B) \\ C(12)-H(12B) \\ N(3)-C(9) \\ \hline \\ C(1)-N(1)-C(11) \\ C(3)-C(2)-C(1) \\ C(3)-C(4)-C(5) \\ N(1)-C(1)-C(2) \\ C(5)-C(6)-C(1) \\ C(6)-C(5)-C(4) \\ C(2)-C(3)-C(4) \\ \hline \\ C(2)-C(3)-C(4) \\ \hline \end{array}$	$\begin{array}{c} 1.352(4)\\ 1.375(4)\\ 1.386(4)\\ 1.406(4)\\ 0.9300\\ 1.417(4)\\ 0.9600\\ 0.9600\\ 1.143(4)\\ 122.3(3)\\ 120.4(4)\\ 116.3(3)\\ 121.2(3)\\ 121.2(3)\\ 121.4(3)\\ 123.1(3)\\ \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6) C(5)-C(6)-H(6) C(6)-C(5)-H(5) C(2)-C(3)-H(3)	$\begin{array}{c} 1.453(4) \\ 1.395(4) \\ 1.415(4) \\ 1.373(3) \\ 0.9300 \\ 1.430(4) \\ 0.9600 \\ 0.9600 \\ 1.127(4) \\ 121.3(3) \\ 119.8 \\ 118.7(3) \\ 121.1(3) \\ 119.4 \\ 119.3 \\ 118.5 \\ (1) \end{array}$	$\begin{array}{c} N(1)-C(12)\\ C(2)-H(2)\\ C(4)-C(7)\\ C(6)-H(6)\\ C(8)-C(7)\\ C(7)-H(7)\\ C(11)-H(11A)\\ C(12)-H(12A)\\ \end{array}$	$\begin{array}{c} 1.455(4)\\ 0.9300\\ 1.422(4)\\ 0.9300\\ 1.367(4)\\ 0.9300\\ 0.9600\\ 0.9600\\ \end{array}$ $\begin{array}{c} 116.4(3)\\ 119.8\\ 125.0(3)\\ 117.6(3)\\ 119.4\\ 119.3\\ 118.5\\ \end{array}$		
$\begin{array}{c} N(1)-C(1) \\ C(2)-C(3) \\ C(4)-C(3) \\ C(1)-C(6) \\ C(5)-H(5) \\ C(8)-C(9) \\ C(11)-H(11B) \\ C(12)-H(12B) \\ N(3)-C(9) \\ \hline \\ C(1)-N(1)-C(11) \\ C(3)-C(2)-C(1) \\ C(3)-C(2)-C(1) \\ C(3)-C(4)-C(5) \\ N(1)-C(1)-C(2) \\ C(5)-C(6)-C(1) \\ C(6)-C(5)-C(4) \\ C(2)-C(3)-C(4) \\ C(7)-C(8)-C(9) \\ \hline \end{array}$	$\begin{array}{c} 1.352(4)\\ 1.375(4)\\ 1.386(4)\\ 1.406(4)\\ 0.9300\\ 1.417(4)\\ 0.9600\\ 0.9600\\ 1.143(4)\\ 122.3(3)\\ 120.4(4)\\ 116.3(3)\\ 121.2(3)\\ 121.2(3)\\ 121.2(3)\\ 121.4(3)\\ 123.1(3)\\ 119.3(3)\\ \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6) C(5)-C(6)-H(6) C(6)-C(5)-H(5) C(2)-C(3)-H(3) C(7)-C(8)-C(10)	$\begin{array}{c} 1.453(4)\\ 1.395(4)\\ 1.415(4)\\ 1.373(3)\\ 0.9300\\ 1.430(4)\\ 0.9600\\ 0.9600\\ 1.127(4)\\ 121.3(3)\\ 119.8\\ 118.7(3)\\ 121.1(3)\\ 119.4\\ 119.3\\ 118.5\\ 125.6(3)\\ \end{array}$	$\begin{array}{c} N(1)-C(12)\\ C(2)-H(2)\\ C(4)-C(7)\\ C(6)-H(6)\\ C(8)-C(7)\\ C(7)-H(7)\\ C(11)-H(11A)\\ C(12)-H(12A)\\ \end{array}$	$\begin{array}{c} 1.455(4)\\ 0.9300\\ 1.422(4)\\ 0.9300\\ 1.367(4)\\ 0.9300\\ 0.9600\\ 0.9600\\ \end{array}$ $\begin{array}{c} 116.4(3)\\ 119.8\\ 125.0(3)\\ 117.6(3)\\ 119.4\\ 119.3\\ 118.5\\ 114.9(4)\\ \end{array}$		
$\begin{array}{c} N(1)-C(1)\\ C(2)-C(3)\\ C(4)-C(3)\\ C(1)-C(6)\\ C(5)-H(5)\\ C(8)-C(9)\\ C(11)-H(11B)\\ C(12)-H(12B)\\ N(3)-C(9)\\ \hline\\ C(1)-N(1)-C(11)\\ C(3)-C(2)-C(1)\\ C(3)-C(2)-C(1)\\ C(3)-C(4)-C(5)\\ N(1)-C(1)-C(2)\\ C(5)-C(6)-C(1)\\ C(6)-C(5)-C(4)\\ C(2)-C(3)-C(4)\\ C(7)-C(8)-C(9)\\ C(8)-C(7)-C(4)\\ \hline\end{array}$	$\begin{array}{c} 1.352(4)\\ 1.375(4)\\ 1.386(4)\\ 1.406(4)\\ 0.9300\\ 1.417(4)\\ 0.9600\\ 0.9600\\ 1.143(4)\\ 122.3(3)\\ 120.4(4)\\ 116.3(3)\\ 121.2(3)\\ 121.2(3)\\ 121.2(3)\\ 121.4(3)\\ 123.1(3)\\ 119.3(3)\\ 132.0(3)\\ \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6) C(5)-C(6)-H(6) C(5)-C(6)-H(6) C(6)-C(5)-H(5) C(2)-C(3)-H(3) C(7)-C(8)-C(10) C(8)-C(7)-H(7)	$\begin{array}{c} 1.453(4)\\ 1.395(4)\\ 1.415(4)\\ 1.373(3)\\ 0.9300\\ 1.430(4)\\ 0.9600\\ 0.9600\\ 1.127(4)\\ 121.3(3)\\ 119.8\\ 118.7(3)\\ 121.1(3)\\ 119.4\\ 119.3\\ 118.5\\ 125.6(3)\\ 114.0\\ \end{array}$	$\begin{array}{c} N(1)-C(12)\\ C(2)-H(2)\\ C(4)-C(7)\\ C(6)-H(6)\\ C(8)-C(7)\\ C(7)-H(7)\\ C(11)-H(11A)\\ C(12)-H(12A)\\ \end{array}$	$\begin{array}{c} 1.455(4)\\ 0.9300\\ 1.422(4)\\ 0.9300\\ 1.367(4)\\ 0.9300\\ 0.9600\\ 0.9600\\ \end{array}$ $\begin{array}{c} 116.4(3)\\ 119.8\\ 125.0(3)\\ 117.6(3)\\ 119.4\\ 119.3\\ 118.5\\ 114.9(4)\\ 114.0\\ \end{array}$		
$\begin{array}{c} N(1)-C(1)\\ C(2)-C(3)\\ C(4)-C(3)\\ C(1)-C(6)\\ C(5)-H(5)\\ C(8)-C(9)\\ C(11)-H(11B)\\ C(12)-H(12B)\\ N(3)-C(9)\\ \hline\\ C(1)-N(1)-C(11)\\ C(3)-C(2)-C(1)\\ C(3)-C(2)-C(1)\\ C(3)-C(4)-C(5)\\ N(1)-C(1)-C(2)\\ C(5)-C(6)-C(1)\\ C(6)-C(5)-C(4)\\ C(2)-C(3)-C(4)\\ C(7)-C(8)-C(9)\\ C(8)-C(7)-C(4)\\ N(1)-C(11)-H(11B)\\ \hline\end{array}$	$\begin{array}{c} 1.352(4)\\ 1.375(4)\\ 1.386(4)\\ 1.406(4)\\ 0.9300\\ 1.417(4)\\ 0.9600\\ 0.9600\\ 1.143(4)\\ 122.3(3)\\ 120.4(4)\\ 116.3(3)\\ 121.2(3)\\ 121.2(3)\\ 121.2(3)\\ 121.4(3)\\ 123.1(3)\\ 119.3(3)\\ 132.0(3)\\ 109.5 \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6) C(5)-C(6)-H(6) C(5)-C(6)-H(6) C(6)-C(5)-H(5) C(2)-C(3)-H(3) C(7)-C(8)-C(10) C(8)-C(7)-H(7) N(1)-C(11)-H(11C)	$\begin{array}{c} 1.453(4)\\ 1.395(4)\\ 1.415(4)\\ 1.373(3)\\ 0.9300\\ 1.430(4)\\ 0.9600\\ 0.9600\\ 1.127(4)\\ 121.3(3)\\ 119.8\\ 118.7(3)\\ 121.1(3)\\ 119.4\\ 119.3\\ 118.5\\ 125.6(3)\\ 114.0\\ 109.5\\ \end{array}$	$\begin{array}{c} N(1)-C(12)\\ C(2)-H(2)\\ C(4)-C(7)\\ C(6)-H(6)\\ C(8)-C(7)\\ C(7)-H(7)\\ C(11)-H(11A)\\ C(12)-H(12A)\\ \end{array}$	$\begin{array}{c} 1.455(4)\\ 0.9300\\ 1.422(4)\\ 0.9300\\ 1.367(4)\\ 0.9300\\ 0.9600\\ 0.9600\\ \end{array}$ $\begin{array}{c} 116.4(3)\\ 119.8\\ 125.0(3)\\ 117.6(3)\\ 119.4\\ 119.3\\ 118.5\\ 114.9(4)\\ 114.0\\ 109.5\\ \end{array}$		
$\begin{array}{c} N(1)-C(1)\\ C(2)-C(3)\\ C(4)-C(3)\\ C(1)-C(6)\\ C(5)-H(5)\\ C(8)-C(9)\\ C(11)-H(11B)\\ C(12)-H(12B)\\ N(3)-C(9)\\ \hline\\ C(1)-N(1)-C(11)\\ C(3)-C(2)-C(1)\\ C(3)-C(2)-C(1)\\ C(3)-C(4)-C(5)\\ N(1)-C(1)-C(2)\\ C(5)-C(6)-C(1)\\ C(6)-C(5)-C(4)\\ C(2)-C(3)-C(4)\\ C(7)-C(8)-C(9)\\ C(8)-C(7)-C(4)\\ N(1)-C(11)-H(11B)\\ N(1)-C(11)-H(11A)\\ \hline\end{array}$	$\begin{array}{c} 1.352(4)\\ 1.375(4)\\ 1.386(4)\\ 1.406(4)\\ 0.9300\\ 1.417(4)\\ 0.9600\\ 0.9600\\ 1.143(4)\\ 122.3(3)\\ 120.4(4)\\ 116.3(3)\\ 121.2(3)\\ 121.2(3)\\ 121.2(3)\\ 121.4(3)\\ 123.1(3)\\ 119.3(3)\\ 132.0(3)\\ 109.5\\ 109.5\\ \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6) C(5)-C(6)-H(6) C(5)-C(6)-H(6) C(6)-C(5)-H(5) C(2)-C(3)-H(3) C(7)-C(8)-C(10) C(8)-C(7)-H(7) N(1)-C(11)-H(11C) H(11B)-C(11)-H(11A)	$\begin{array}{c} 1.453(4)\\ 1.395(4)\\ 1.373(3)\\ 0.9300\\ 1.430(4)\\ 0.9600\\ 0.9600\\ 1.127(4)\\ 121.3(3)\\ 119.8\\ 118.7(3)\\ 121.1(3)\\ 119.4\\ 119.3\\ 118.5\\ 125.6(3)\\ 114.0\\ 109.5\\ 109.5\\ \end{array}$	$\begin{array}{c} N(1)-C(12)\\ C(2)-H(2)\\ C(4)-C(7)\\ C(6)-H(6)\\ C(8)-C(7)\\ C(7)-H(7)\\ C(11)-H(11A)\\ C(12)-H(12A)\\ \end{array}$	$\begin{array}{c} 1.455(4)\\ 0.9300\\ 1.422(4)\\ 0.9300\\ 1.367(4)\\ 0.9300\\ 0.9600\\ 0.9600\\ \end{array}$ $\begin{array}{c} 116.4(3)\\ 119.8\\ 125.0(3)\\ 117.6(3)\\ 119.4\\ 119.3\\ 118.5\\ 114.9(4)\\ 114.0\\ 109.5\\ 109.5\\ \end{array}$		
$\begin{array}{c} N(1)-C(1)\\ C(2)-C(3)\\ C(4)-C(3)\\ C(1)-C(6)\\ C(5)-H(5)\\ C(8)-C(9)\\ C(11)-H(11B)\\ C(12)-H(12B)\\ N(3)-C(9)\\ \hline\\ C(1)-N(1)-C(11)\\ C(3)-C(2)-C(1)\\ C(3)-C(2)-C(1)\\ C(3)-C(4)-C(5)\\ N(1)-C(1)-C(2)\\ C(5)-C(6)-C(1)\\ C(6)-C(5)-C(4)\\ C(2)-C(3)-C(4)\\ C(7)-C(8)-C(9)\\ C(8)-C(7)-C(4)\\ N(1)-C(11)-H(11B)\\ N(1)-C(11)-H(11B)\\ N(1)-C(12)-H(12B)\\ \hline\end{array}$	$\begin{array}{c} 1.352(4)\\ 1.375(4)\\ 1.386(4)\\ 1.406(4)\\ 0.9300\\ 1.417(4)\\ 0.9600\\ 0.9600\\ 1.143(4)\\ 122.3(3)\\ 120.4(4)\\ 116.3(3)\\ 121.2(3)\\ 121.2(3)\\ 121.2(3)\\ 121.4(3)\\ 123.1(3)\\ 119.3(3)\\ 132.0(3)\\ 109.5\\ 109.5\\ 109.5\\ \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6) C(5)-C(6)-H(6) C(5)-C(6)-H(6) C(6)-C(5)-H(5) C(2)-C(3)-H(3) C(7)-C(8)-C(10) C(8)-C(7)-H(7) N(1)-C(11)-H(11C) H(11B)-C(11)-H(11A) N(1)-C(12)-H(12C)	$\begin{array}{c} 1.453(4)\\ 1.395(4)\\ 1.373(3)\\ 0.9300\\ 1.430(4)\\ 0.9600\\ 0.9600\\ 1.127(4)\\ \hline\\ 121.3(3)\\ 119.8\\ 118.7(3)\\ 121.1(3)\\ 119.4\\ 119.3\\ 118.5\\ 125.6(3)\\ 114.0\\ 109.5\\ 109.5\\ 109.5\\ \hline\end{array}$	$\begin{array}{c} N(1)-C(12)\\ C(2)-H(2)\\ C(4)-C(7)\\ C(6)-H(6)\\ C(8)-C(7)\\ C(7)-H(7)\\ C(11)-H(11A)\\ C(12)-H(12A)\\ \end{array}$	$\begin{array}{c} 1.455(4)\\ 0.9300\\ 1.422(4)\\ 0.9300\\ 1.367(4)\\ 0.9300\\ 0.9600\\ 0.9600\\ \end{array}$ $\begin{array}{c} 116.4(3)\\ 119.8\\ 125.0(3)\\ 117.6(3)\\ 119.4\\ 119.3\\ 118.5\\ 114.9(4)\\ 114.0\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ \end{array}$		
$\begin{array}{c} N(1)-C(1)\\ C(2)-C(3)\\ C(4)-C(3)\\ C(1)-C(6)\\ C(5)-H(5)\\ C(8)-C(9)\\ C(11)-H(11B)\\ C(12)-H(12B)\\ N(3)-C(9)\\ \hline\\ C(1)-N(1)-C(11)\\ C(3)-C(2)-C(1)\\ C(3)-C(2)-C(1)\\ C(3)-C(4)-C(5)\\ N(1)-C(1)-C(2)\\ C(5)-C(6)-C(1)\\ C(6)-C(5)-C(4)\\ C(2)-C(3)-C(4)\\ C(7)-C(8)-C(9)\\ C(8)-C(7)-C(4)\\ N(1)-C(11)-H(11B)\\ N(1)-C(11)-H(11B)\\ N(1)-C(12)-H(12B)\\ N(1)-C(12)-H(12B)\\ N(1)-C(12)-H(12A)\\ \hline\end{array}$	$\begin{array}{c} 1.352(4)\\ 1.375(4)\\ 1.386(4)\\ 1.406(4)\\ 0.9300\\ 1.417(4)\\ 0.9600\\ 0.9600\\ 1.143(4)\\ 122.3(3)\\ 120.4(4)\\ 116.3(3)\\ 121.2(3)\\ 121.2(3)\\ 121.2(3)\\ 121.4(3)\\ 123.1(3)\\ 119.3(3)\\ 132.0(3)\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ \end{array}$	$\begin{array}{c} \textbf{Chromophore 2} \\ N(1)-C(11) \\ C(2)-C(1) \\ C(4)-C(5) \\ C(6)-C(5) \\ C(3)-H(3) \\ C(8)-C(10) \\ C(11)-H(11C) \\ C(12)-H(12C) \\ C(10)-N(2) \\ \end{array}$	$\begin{array}{c} 1.453(4)\\ 1.395(4)\\ 1.373(3)\\ 0.9300\\ 1.430(4)\\ 0.9600\\ 0.9600\\ 1.127(4)\\ \hline\\ 121.3(3)\\ 119.8\\ 118.7(3)\\ 121.1(3)\\ 119.4\\ 119.3\\ 118.5\\ 125.6(3)\\ 114.0\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ \hline\end{array}$	$\begin{array}{c} N(1)-C(12)\\ C(2)-H(2)\\ C(4)-C(7)\\ C(6)-H(6)\\ C(8)-C(7)\\ C(7)-H(7)\\ C(11)-H(11A)\\ C(12)-H(12A)\\ \end{array}$	$\begin{array}{c} 1.455(4)\\ 0.9300\\ 1.422(4)\\ 0.9300\\ 1.367(4)\\ 0.9300\\ 0.9600\\ 0.9600\\ \end{array}$ $\begin{array}{c} 116.4(3)\\ 119.8\\ 125.0(3)\\ 117.6(3)\\ 119.4\\ 119.3\\ 118.5\\ 114.9(4)\\ 114.0\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ \end{array}$		
$\begin{array}{c} N(1)-C(1)\\ C(2)-C(3)\\ C(4)-C(3)\\ C(1)-C(6)\\ C(5)-H(5)\\ C(8)-C(9)\\ C(11)-H(11B)\\ C(12)-H(12B)\\ N(3)-C(9)\\ \end{array}$ $\begin{array}{c} C(1)-N(1)-C(11)\\ C(3)-C(2)-C(1)\\ C(3)-C(2)-C(1)\\ C(3)-C(4)-C(5)\\ N(1)-C(1)-C(2)\\ C(5)-C(6)-C(1)\\ C(6)-C(5)-C(4)\\ C(2)-C(3)-C(4)\\ C(7)-C(8)-C(9)\\ C(8)-C(7)-C(4)\\ N(1)-C(11)-H(11B)\\ N(1)-C(11)-H(11B)\\ N(1)-C(12)-H(12B)\\ N(1)-C(12)-H(12A)\\ N(2)-C(10)-C(8)\\ \end{array}$	$\begin{array}{c} 1.352(4)\\ 1.375(4)\\ 1.386(4)\\ 1.406(4)\\ 0.9300\\ 1.417(4)\\ 0.9600\\ 0.9600\\ 1.143(4)\\ 122.3(3)\\ 120.4(4)\\ 116.3(3)\\ 121.2(3)\\ 121.2(3)\\ 121.2(3)\\ 121.4(3)\\ 123.1(3)\\ 119.3(3)\\ 132.0(3)\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ 177.7(5)\\ \end{array}$	Chromophore 2 N(1)-C(11) C(2)-C(1) C(4)-C(5) C(6)-C(5) C(3)-H(3) C(8)-C(10) C(11)-H(11C) C(12)-H(12C) C(10)-N(2) C(1)-N(1)-C(12) C(3)-C(2)-H(2) C(3)-C(2)-H(2) C(3)-C(4)-C(7) N(1)-C(1)-C(6) C(5)-C(6)-H(6) C(5)-C(6)-H(6) C(6)-C(5)-H(5) C(2)-C(3)-H(3) C(7)-C(8)-C(10) C(8)-C(7)-H(7) N(1)-C(11)-H(11C) H(11B)-C(11)-H(11A) N(1)-C(12)-H(12C) H(12B)-C(12)-H(12A) N(3)-C(9)-C(8)	$\begin{array}{c} 1.453(4)\\ 1.395(4)\\ 1.373(3)\\ 0.9300\\ 1.430(4)\\ 0.9600\\ 0.9600\\ 1.127(4)\\ 121.3(3)\\ 119.8\\ 118.7(3)\\ 121.1(3)\\ 119.4\\ 119.3\\ 118.5\\ 125.6(3)\\ 114.0\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ 178.0(4)\\ \end{array}$	$\begin{array}{c} N(1)-C(12)\\ C(2)-H(2)\\ C(4)-C(7)\\ C(6)-H(6)\\ C(8)-C(7)\\ C(7)-H(7)\\ C(11)-H(11A)\\ C(12)-H(12A)\\ \end{array}$	$\begin{array}{c} 1.455(4)\\ 0.9300\\ 1.422(4)\\ 0.9300\\ 1.367(4)\\ 0.9300\\ 0.9600\\ 0.9600\\ \end{array}$ $\begin{array}{c} 116.4(3)\\ 119.8\\ 125.0(3)\\ 117.6(3)\\ 119.4\\ 119.3\\ 118.5\\ 114.9(4)\\ 114.0\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ 109.5\\ \end{array}$		

Charaman have 2							
$\begin{array}{l} N(2)-C(4) \\ C(1)-C(6) \\ C(7)-C(8) \\ C(6)-H(6) \\ C(5)-C(4) \\ O(2)-C(11) \\ C(10)-O(1) \\ C(14)-H(14) \\ C(9)-N(1) \\ C(13)-H(13B) \\ C(11)-H(11A) \\ C(12)-H(12A) \end{array}$	$\begin{array}{c} 1.3568(17)\\ 1.405(2)\\ 1.3550(19)\\ 0.9300\\ 1.4147(19)\\ 1.452(2)\\ 1.1990(19)\\ 0.9600\\ 1.141(2)\\ 0.9600\\ 0.9700\\ 0.9600\\ \end{array}$	$\begin{array}{l} N(2)-C(14) \\ C(1)-C(2) \\ C(7)-H(7) \\ C(2)-C(3) \\ C(5)-H(5) \\ C(8)-C(9) \\ C(3)-C(4) \\ C(14)-H(14C) \\ C(13)-H(13A) \\ C(11)-C(12) \\ C(12)-H(12C) \end{array}$	$\begin{array}{c} 1.442(2) \\ 1.4059(18) \\ 0.9300 \\ 1.3630(19) \\ 0.9300 \\ 1.429(2) \\ 1.409(2) \\ 0.9600 \\ 0.9600 \\ 1.466(3) \\ 0.9600 \end{array}$	N(2)-C(13) C(1)-C(7) C(6)-C(5) C(2)-H(2) O(2)-C(10) C(8)-C(10) C(3)-H(3) C(14)-H(14B) C(13)-H(13C) C(11)-H(11B) C(12)-H(12B)	$\begin{array}{c} 1.4564(19)\\ 1.4316(19)\\ 1.371(2)\\ 0.9300\\ 1.3418(18)\\ 1.481(2)\\ 0.9300\\ 0.9600\\ 0.9600\\ 0.9700\\ 0.960\end{array}$		
$\begin{array}{c} C(4)-N(2)-C(14)\\ C(6)-C(1)-C(2)\\ C(8)-C(7)-C(1)\\ C(5)-C(6)-C(1)\\ C(3)-C(2)-C(1)\\ C(6)-C(5)-C(4)\\ C(10)-O(2)-C(11)\\ C(9)-C(8)-C(10)\\ O(2)-C(10)-C(8)\\ C(4)-C(3)-H(3)\\ H(14)-C(14)-H(14C)\\ H(14C)-C(14)-H(14C)\\ H(14C)-C(13)-H(13C)\\ H(13A)-C(13)-H(13B)\\ O(2)-C(11)-H(11B)\\ C(12)-C(11)-H(11B)\\ C(12)-C(12)-H(12B)\\ H(12C)-C(12)-H(12B)\\ H(12C)-C(4)-C(5)\\ \end{array}$	121.07(12) $115.95(12)$ $132.63(15)$ $122.04(13)$ $122.80(13)$ $121.45(13)$ $117.12(15)$ $117.78(13)$ $111.85(14)$ 119.4 109.5 109.5 109.5 109.5 109.2 109.2 109.2 109.5	$\begin{array}{c} C(4)-N(2)-C(13)\\ C(6)-C(1)-C(7)\\ C(8)-C(7)-H(7)\\ C(5)-C(6)-H(6)\\ C(3)-C(2)-H(2)\\ C(6)-C(5)-H(5)\\ C(7)-C(8)-C(9)\\ O(1)-C(10)-O(2)\\ C(2)-C(3)-C(4)\\ N(2)-C(14)-H(14)\\ N(2)-C(14)-H(14B)\\ N(1)-C(9)-C(8)\\ H(13A)-C(13)-H(13C)\\ H(13C)-C(13)-H(13B)\\ C(12)-C(11)-H(11B)\\ H(11B)-C(11)-H(11B)\\ H(11B)-C(12)-H(12B)\\ H(12B)-C(12)-H(12A)\\ C(3)-C(4)-C(5)\\ \end{array}$	$120.95(13) \\ 126.39(12) \\ 113.7 \\ 119.0 \\ 118.6 \\ 119.3 \\ 123.62(14) \\ 123.94(15) \\ 121.19(13) \\ 109.5 \\ 116.56(13) \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ $	$\begin{array}{c} C(14)-N(2)-C(13)\\ C(2)-C(1)-C(7)\\ C(1)-C(7)-H(7)\\ C(1)-C(6)-H(6)\\ C(1)-C(2)-H(2)\\ C(4)-C(5)-H(5)\\ C(7)-C(8)-C(10)\\ O(1)-C(10)-C(8)\\ C(2)-C(3)-H(3)\\ N(2)-C(14)-H(14C)\\ H(14)-C(14)-H(14B)\\ N(2)-C(13)-H(13B)\\ O(2)-C(13)-H(13B)\\ O(2)-C(11)-H(13B)\\ O(2)-C(11)-H(11A)\\ C(11)-C(12)-H(12C)\\ C(11)-C(12)-H(12A)\\ N(2)-C(4)-C(3)\\ \end{array}$	117.42(13) 117.67(13) 113.7 119.0 118.6 119.3 118.60(14) 124.21(14) 119.4 109.5 109.5 109.5 109.5 112.21(16) 109.5		
$\begin{array}{c} C(7)-C(8)\\ O(2)-C(10)\\ N(1)-C(13)\\ C(4)-C(3)\\ O(1)-C(10)\\ C(6)-C(1)\\ C(5)-H(5)\\ C(3)-H(3)\\ C(13)-H(13C)\\ C(12)-H(12C)\\ C(11)-H(11C) \end{array}$	$\begin{array}{c} 1.352(2)\\ 1.343(2)\\ 1.443(2)\\ 1.410(2)\\ 1.197(2)\\ 1.396(2)\\ 0.9300\\ 0.9300\\ 0.9600\\ 0.9600\\ 0.9600\\ \end{array}$	Chromophore 4 C(7)–C(1) O(2)–C(11) N(1)–C(12) C(8)–C(9) C(9)–N(2) C(6)–H(6) C(2)–C(3) C(13)–H(13A) C(12)–H(12A) C(11)–H(11A)	$\begin{array}{c} 1.438(2) \\ 1.437(2) \\ 1.445(2) \\ 1.445(2) \\ 1.145(2) \\ 0.9300 \\ 1.362(2) \\ 0.9600 \\ 0.9600 \\ 0.9600 \end{array}$	C(7)-H(7) N(1)-C(4) C(4)-C(5) C(8)-C(10) C(6)-C(5) C(1)-C(2) C(2)-H(2) C(13)-H(13B) C(12)-H(12B) C(11)-H(11B)	$\begin{array}{c} 0.9300\\ 1.361(2)\\ 1.404(2)\\ 1.473(2)\\ 1.366(2)\\ 1.399(2)\\ 0.9300\\ 0.9600\\ 0.9600\\ 0.9600\\ 0.9600\\ \end{array}$		
$\begin{array}{c} C(8)-C(7)-C(1)\\ C(10)-O(2)-C(11)\\ C(13)-N(1)-C(12)\\ C(5)-C(4)-C(3)\\ C(9)-C(8)-C(10)\\ C(5)-C(6)-H(6)\\ C(6)-C(1)-C(7)\\ C(6)-C(5)-H(5)\\ C(3)-C(2)-H(2)\\ O(1)-C(10)-C(8)\\ C(2)-C(3)-H(3)\\ N(1)-C(13)-H(13B)\\ H(13A)-C(13)-H(13C)\\ N(1)-C(12)-H(12B)\\ H(12A)-C(12)-H(12C)\\ O(2)-C(11)-H(11B)\\ H(11A)-C(11)-H(11C)\\ \end{array}$	$\begin{array}{c} 132.04(16)\\ 116.09(15)\\ 118.06(14)\\ 116.41(14)\\ 117.02(14)\\ 118.8\\ 118.03(15)\\ 119.4\\ 119.1\\ 125.15(16)\\ 119.1\\ 109.5\\ 10$	$\begin{array}{c} C(8)-C(7)-H(7)\\ C(4)-N(1)-C(13)\\ N(1)-C(4)-C(5)\\ C(7)-C(8)-C(9)\\ N(2)-C(9)-C(8)\\ C(1)-C(6)-H(6)\\ C(2)-C(1)-C(7)\\ C(4)-C(5)-H(5)\\ C(1)-C(2)-H(2)\\ O(2)-C(10)-C(8)\\ C(4)-C(3)-H(3)\\ H(13A)-C(13)-H(13B)\\ H(13B)-C(13)-H(13C)\\ H(12A)-C(12)-H(12B)\\ H(12B)-C(12)-H(12C)\\ H(11A)-C(11)-H(11B)\\ H(11B)-C(11)-H(11C)\\ \end{array}$	$\begin{array}{c} 114.0\\ 120.85(15)\\ 122.15(15)\\ 124.43(15)\\ 179.6(2)\\ 118.8\\ 125.57(15)\\ 119.4\\ 119.1\\ 112.08(15)\\ 119.1\\ 109.5\\ 10$	$\begin{array}{c} C(1)-C(7)-H(7)\\ C(4)-N(1)-C(12)\\ N(1)-C(4)-C(3)\\ C(7)-C(8)-C(10)\\ C(5)-C(6)-C(1)\\ C(6)-C(1)-C(2)\\ C(6)-C(5)-C(4)\\ C(3)-C(2)-C(1)\\ O(1)-C(10)-O(2)\\ C(2)-C(3)-C(4)\\ N(1)-C(13)-H(13A)\\ N(1)-C(13)-H(13C)\\ N(1)-C(12)-H(12A)\\ N(1)-C(12)-H(12C)\\ O(2)-C(11)-H(11A)\\ O(2)-C(11)-H(11C)\\ \end{array}$	114.0 121.09(15) 121.44(15) 118.55(15) 122.44(16) 116.40(14) 121.17(16) 121.81(16) 122.75(16) 121.74(16) 109.5 109.5 109.5 109.5 109.5		

VI. View of C–H... π interactions



Fig. S10: View of C–H... π interactions in chromophore **1**



Fig. S11: View of C–H... π interactions in chromophore 3



Fig. S12: View of C–H... π interactions in chromophore **4**

VII. Orientation of molecules in unit cell



Fig. S13: Orientation of chromophores (a) 1, (b) 2, (c) 3 and (d) 4 in unit cell.

VIII. Thermal activation energy plots



Fig. S14: Thermal activation energy plots of (a) chromophore 1, (b) chromophore 2, (c) chromophore 3 and (d) chromophore 4.

IX. UV-Vis. absorption spectra in different solvents



Fig. S15: Absorption spectra of (a) chromophore **1**, (b) chromophore **2**, (c) chromophore **3** and (d) chromophore **4**; in different solvents with molar concentration 1.0×10^{-5} M.

X. Fluorescence spectra in different solvents



Fig. S16: Fluorescence spectra of (a) chromophore **1**, (b) chromophore **2**, (c) chromophore **3** and (d) chromophore **4**; in different solvents with molar concentration 1.0×10^{-5} M.

XI. Lippert-Mataga plots



Fig. S17: Lippert-Mataga plots of Stokes shift against the solvent polarity function (Δf) for (a) chromophore 1, (b) chromophore 2, (c) chromophore 3 and (d) chromophore 4.