

## ELECTRONIC SUPPLEMENTARY INFORMATION

### **Control of crystal structures of fluorescent two-component supramolecular systems by varying substituents and their positions**

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**Table ESI-1.** Crystallographic data for complexes I-VI

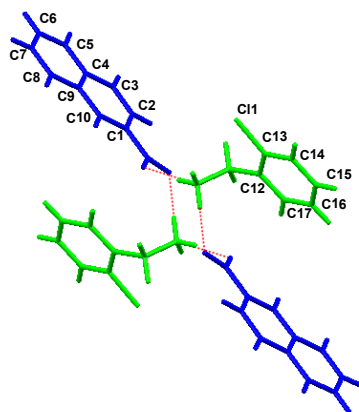
	I	II	III
Empirical formula	C <sub>11</sub> H <sub>8</sub> O <sub>2</sub> ·C <sub>7</sub> H <sub>8</sub> ClN	C <sub>11</sub> H <sub>8</sub> O <sub>2</sub> ·C <sub>7</sub> H <sub>8</sub> ClN	C <sub>11</sub> H <sub>8</sub> O <sub>2</sub> ·C <sub>7</sub> H <sub>8</sub> BrN
Formula weight	313.77	313.77	358.23
Crystal system	monoclinic	orthorhombic	triclinic
Space group	<i>C2/c</i>	<i>Pbca</i>	<i>P</i> $\bar{1}$
Symmetry codes	<i>x, y, z; -x, y, -z+1/2; x+1/2, y+1/2, z; -x+1/2, y+1/2, -z+1/2; -x, -y, -z; x, -y, z-1/2; -x+1/2, y+1/2, -z; x+1/2, -y+1/2, z-1/2</i>	<i>x, y, z; -x+1/2, -y, z+1/2; -x, y+1/2, -z+1/2; x+1/2, -y+1/2, -z; -x, -y, -z; x-1/2, y, -z-1/2; x, -y-1/2, z-1/2; -x-1/2, y-1/2, z</i>	<i>x, y, z; -x, -y, -z</i>
<i>a</i> / Å	18.671(2)	10.5204(7)	4.6370(18)
<i>b</i> / Å	6.0403(6)	8.7184(6)	11.658(4)
<i>c</i> / Å	29.098(3)	33.531(2)	15.392(5)
<i>α</i> / deg	90.00	90.00	67.925(12)
<i>β</i> / deg	106.031(4)	90.00	82.161(15)
<i>γ</i> / deg	90.00	90.00	85.996(18)
<i>Z</i>	8	8	2
<i>D<sub>c</sub></i> / g cm <sup>-3</sup>	1.322	1.355	1.558
<i>V</i> / Å <sup>3</sup>	3154.0(6)	3075.5(3)	763.7(5)
<i>μ</i> (Mo Kα) / mm <sup>-1</sup>	0.248	0.255	2.698
No. of reflections			
measured	8452	17697	5471
unique	3107	3610	3268
<i>I</i> > 2.0σ( <i>I</i> )	2667	2827	2811
<i>R</i> ( <i>I</i> > 2.0σ( <i>I</i> ))	0.0442	0.0498	0.0645
<i>R</i> (all data)	0.0511	0.0647	0.0757
<i>T</i> / K	93(2)	93(2)	100(2)
CCDC code	965542	965543	965544

	IV	V	VI
Empirical formula	C <sub>11</sub> H <sub>8</sub> O <sub>2</sub> ·C <sub>7</sub> H <sub>8</sub> BrN	C <sub>11</sub> H <sub>8</sub> O <sub>2</sub> ·C <sub>8</sub> H <sub>11</sub> N	C <sub>11</sub> H <sub>8</sub> O <sub>2</sub> ·C <sub>8</sub> H <sub>11</sub> N
Formula weight	358.23	293.35	293.35
Crystal system	orthorhombic	monoclinic	monoclinic
Space group	<i>Pbca</i>	<i>C2/c</i>	<i>P2<sub>1</sub>/c</i>
Symmetry codes	$x, y, z; -x+1/2, -y, z+1/2; -x, y+1/2, -z+1/2; x+1/2, -y+1/2, -z; -x, -y, -z; x-1/2, y, -z-1/2; x, -y-1/2, z-1/2; -x-1/2, y-1/2, z$	$x, y, z; -x, y, -z+1/2; x+1/2, y+1/2, z; -x+1/2, y+1/2, -z+1/2; -x, -y, -z; x, -y, z-1/2; -x+1/2, y+1/2, -z; x+1/2, -y+1/2, z-1/2$	$x, y, z; -x, y+1/2, -z+1/2; -x, -y, -z; x, -y-1/2, z-1/2$
<i>a</i> / Å	10.6279(9)	18.404(5)	15.604(4)
<i>b</i> / Å	8.7139(7)	6.0250(15)	6.2630(14)
<i>c</i> / Å	33.989(3)	28.832(8)	15.601(4)
<i>α</i> / deg	90.00	90.00	90.00
<i>β</i> / deg	90.00	104.628(3)	90.680(3)
<i>γ</i> / deg	90.00	90.00	90.00
<i>Z</i>	8	8	4
<i>D<sub>c</sub></i> / g cm <sup>-3</sup>	1.512	1.260	1.278
<i>V</i> / Å <sup>3</sup>	3147.7(4)	3093.4(14)	1524.5(6)
<i>μ</i> (Mo Kα) / mm <sup>-1</sup>	2.618	0.081	0.083
No. of reflections			
measured	17795	7027	11871
unique	3586	3124	4208
<i>I</i> > 2.0σ( <i>I</i> )	2312	1631	3501
<i>R</i> ( <i>I</i> > 2.0σ( <i>I</i> ))	0.0524	0.0537	0.0433
<i>R</i> (all data)	0.0913	0.1177	0.0526
<i>T</i> / K	100(2)	100(2)	100(2)
CCDC code	965545	965546	965547

**Table ESI-2. Interaction of complex I.**

	Distance (Å)	Interaction	Gamma* (Deg)
<i>A</i>	3.417(2)	C(8)-H... $\pi$ (C4-C5-C6-C7-C8-C9)	6.33
<i>B</i>	3.760(2)	C(3)-H... $\pi$ (C12-C13-C14-C15-C16-C17)	13.88
<i>C</i>	3.454(2)	C(14)-H... $\pi$ (C1-C2-C3-C4-C9-C10)	9.48
<i>D</i>	3.585(3)	C(15)-H... $\pi$ (C4-C5-C6-C7-C8-C9)	6.96
<i>E</i>	3.4214(10)	Cl(1)...Cl(1)	

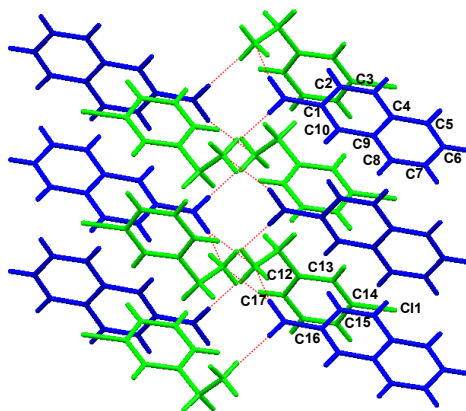
\*Angle C-H vector and normal to  $\pi$  plane



**Table ESI-3. Interaction of complex II.**

	Distance (Å)	Interaction	Gamma* (Deg)
<i>A</i>	3.576(2)	C(8)-H... $\pi$ (C1-C2-C3-C4-C9-C10)	8.41
<i>B</i>	3.5949(18)	C(18)-H... $\pi$ (C12-C13-C14-C15-C16-C17)	7.09
<i>C</i>	3.5857(13)	Cl(1)... $\pi$ (C4-C5-C6-C7-C8-C9)	7.11

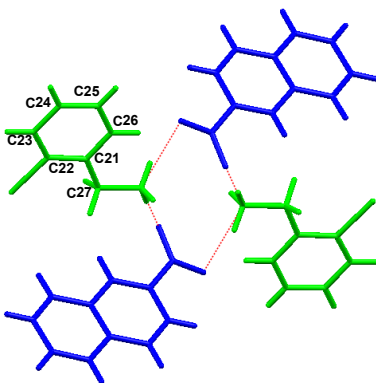
\*Angle C-H (or Cl) vector and normal to  $\pi$  plane



**Table ESI-4.** Interaction of complex **III**.

	Distance (Å)	Interaction	Gamma* (Deg)
<i>A</i>	3.373(6)	C(27)-H... $\pi$ (C21-C22-C23-C24-C25-C26)	1.74

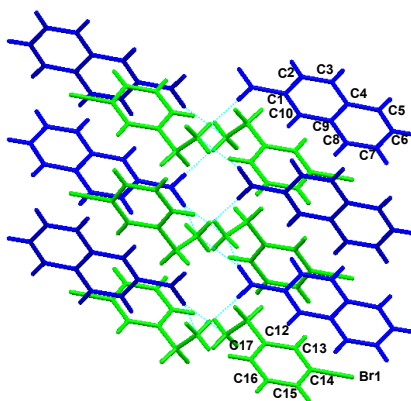
\*Angle C-H vector and normal to  $\pi$  plane



**Table ESI-5.** Interaction of complex **IV**.

	Distance (Å)	Interaction	Gamma* (Deg)
<i>A</i>	3.570(4)	C(8)-H... $\pi$ (C1-C2-C3-C4-C9-C10)	7.92
<i>B</i>	3.568(3)	C(18)-H... $\pi$ (C12-C13-C14-C15-C16-C17)	4.41
<i>C</i>	3.6807 (19)	Br(1)... $\pi$ (C5-C6-C7-C8-C10-C9)	6.81

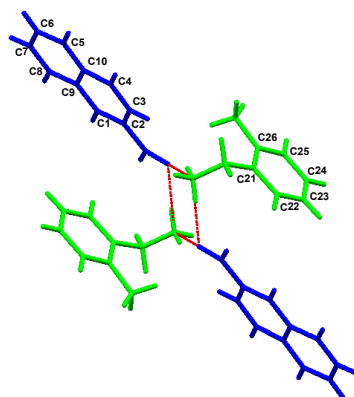
\*Angle C-H (or Br) vector and normal to  $\pi$  plane



**Table ESI-6.** Interaction of complex V.

	Distance (Å)	Interaction	Gamma* (Deg)
<i>A</i>	3.370(3)	C(8)-H... $\pi$ (C5-C6-C7-C8-C9-C10)	6.34
<i>B</i>	3.732(3)	C(4)-H... $\pi$ (C21-C22-C23-C24-C25-C26)	17.70
<i>C</i>	3.424(3)	C(23)-H... $\pi$ (C1-C2-C3-C4-C5-C6)	9.18

\*Angle C-H vector and normal to  $\pi$  plane



**Table ESI-7.** Interaction of complex VI.

	Distance (Å)	Interaction	Gamma* (Deg)
<i>A</i>	3.6113(15)	C(3)-H... $\pi$ (C5-C6-C7-C8-C9-C10)	16.90
<i>B</i>	3.7427(16)	C(28)-H... $\pi$ (C1-C2-C3-C4-C10-C9)	6.60
<i>C</i>	3.3959(15)	C(8)-H... $\pi$ (C21-C22-C23-C24-C25-C26)	1.80
<i>D</i>	3.4249(15)	C(27)-H... $\pi$ (C21-C22-C23-C24-C25-C26)	13.28

\*Angle C-H vector and normal to  $\pi$  plane

