

## Electronic Supplementary Information

### Photophysical Properties of a New Series of Water Soluble Iridium Bisterpyridine Complexes Functionalised at the 4' Position

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**Table S1** Crystallographic Data for **2**, **3**, **4**

Compound	<b>2</b>	<b>3</b>	<b>4</b>
Chemical formula	C <sub>48</sub> H <sub>40</sub> F <sub>18</sub> IrN <sub>8</sub> O <sub>2</sub> P <sub>3</sub>	C <sub>47</sub> H <sub>39</sub> F <sub>18</sub> IrN <sub>9</sub> OP <sub>3</sub>	C <sub>45</sub> H <sub>39</sub> F <sub>18</sub> IrN <sub>9</sub> OP <sub>3</sub>
Formula Mass	1387.99	1372.98	1348.96
Crystal system	Monoclinic	Monoclinic	Monoclinic
<i>a</i> /Å	14.7462(9)	14.7636(4)	15.579(9)
<i>b</i> /Å	16.4284(9)	16.2915(5)	16.280(7)
<i>c</i> /Å	21.4266(12)	21.4687(5)	21.289(12)
$\alpha$ /°	90.00	90.00	90.00
$\beta$ /°	106.021(3)	105.4910(10)	104.50(3)
$\gamma$ /°	90.00	90.00	90.00
Unit cell volume/Å <sup>3</sup>	4989.1(5)	4976.1(2)	5228(5)
Temperature/K	150(2)	150(2)	150(2)
Space group	<i>C2/c</i>	<i>C2/c</i>	<i>C2/c</i>
No. of formula units per unit cell, <i>Z</i>	4	4	4
No. of reflections measured	17391	27970	18677
No. of independent reflections	4395	4373	4592
<i>R</i> <sub>int</sub>	0.0507	0.0567	0.1027
Final <i>R</i> <sub><i>i</i></sub> values ( <i>I</i> > 2σ( <i>I</i> ))	0.0270	0.0242	0.0519
Final <i>wR</i> ( <i>F</i> <sup>2</sup> ) values ( <i>I</i> > 2σ( <i>I</i> ))	0.0781	0.0554	0.1050
Final <i>R</i> <sub><i>i</i></sub> values (all data)	0.0310	0.0279	0.0876
Final <i>wR</i> ( <i>F</i> <sup>2</sup> ) values (all data)	0.0843	0.0569	0.1197