



Supporting Information

© Wiley-VCH 2005

69451 Weinheim, Germany

# White light emission from an assembly comprising a blue emitting iridium and a red emitting europium complex

*Paolo Coppo, Marco Duati, Valery N. Kozhevnikov, Johannes W. Hofstraat, and Luisa De Cola\**

## Experimental details

The emission quantum yields were measured in deaerated solutions, using Quinine bisulphate in 0.5 M H<sub>2</sub>SO<sub>4</sub> as standard for the Iridium complexes **1** and **1a** and [Ru(bpy)<sub>3</sub>]Cl<sub>2</sub> in degassed water solutions for complexes **2**, **2a** and **3**. The UV-Vis absorption spectra were recorded on a Cary 4 UV-visible spectrophotometer. Recording of the emission spectra was performed with a SPEX Fluorolog spectrofluorometer. The emission spectra were corrected for monochromator and photomultiplier efficiency and for xenon lamp stability. Lifetimes were determined using a Coherent Infinity Nd:YAG-XPO laser (1 ns pulses FWHM) and a Hamamatsu C5680-21 streak camera equipped with a Hamamatsu M5677 low-speed single-sweep unit.

The IR spectra were recorded on a Biorad FTS-7 FTIR system in KBr pellets.

Solvents for reactions were distilled prior to use. Solvents for spectroscopy were of a spectroscopic grade and used as purchased. Deuterated solvents were purchased from Cambridge Isotopes in sealed vials and used as received.

## Complex 1

Complex **1** was prepared according to a previously published procedure<sup>5</sup> and purified by chromatography over silica gel, using CH<sub>3</sub>CN-H<sub>2</sub>O-CH<sub>3</sub>OH mixtures to elute.

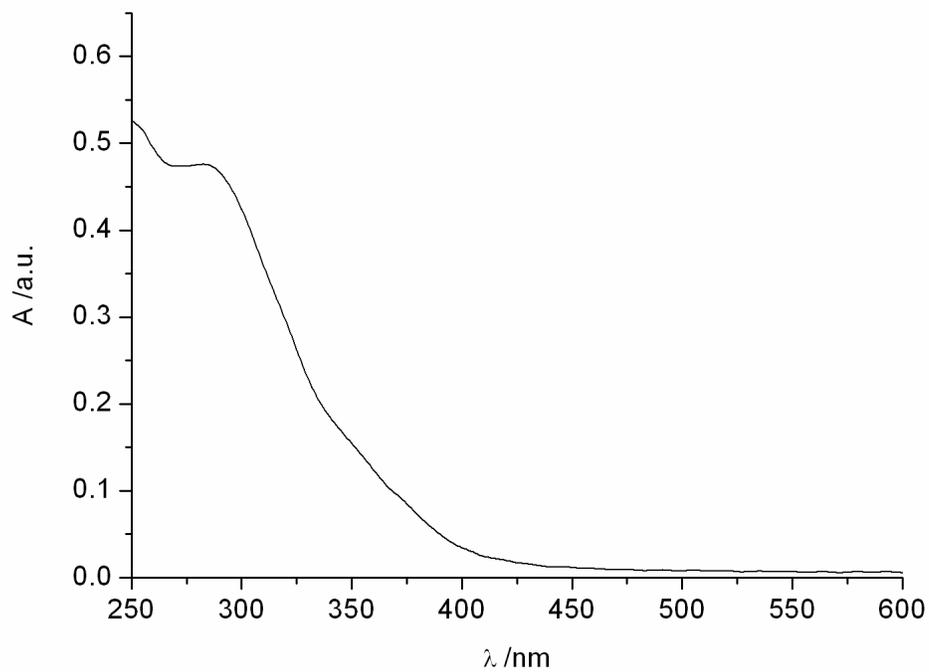
<sup>1</sup>H NMR in CDCl<sub>3</sub>:  $\sigma$  = 8.49 (d, J = 8Hz, 2Hz, 2H, aromatics); 8.31 (dd, J = 8Hz, 2Hz, 2H, aromatics); 8.13 (m, 3H, aromatics); 7.86 (m, 4H, aromatics); 7.42 (dd, J= 8Hz, 2Hz, 2H, aromatics); 7.28 (d, J = 8Hz, 1H, aromatic); 7.10 (dd, J = 8Hz 2Hz, 1H, aromatic); 7.00 (dd, J = 8Hz, 2Hz, 1H, aromatic); 6.55 (dd, J = 8Hz, 2Hz, 2H, aromatic); 5.75 (d, J = 8Hz, 1H, aromatic) 5.68 ppm (d, J = 8Hz, 1H, aromatic).

<sup>13</sup>C NMR in CD<sub>3</sub>OD:  $\sigma$  = 166.44 (C); 166.30 (C); 165.71 (C); 164.78 (C); 163.94 (C); 163.25 (C); 161.52 (C); 159.08 (C); 154.03 (C); 151.82 (C); 151.01 (CH); 150.09 (CH); 141.01 (CH); 140.03 (CH); 139.65 (CH); 138.97 (C); 134.84 (C); 130.53 (CH); 129.24 (C); 126.98 (CH); 124.59 (CH); 124.38 (CH); 122.97 CH); 114.89 ppm (CH).

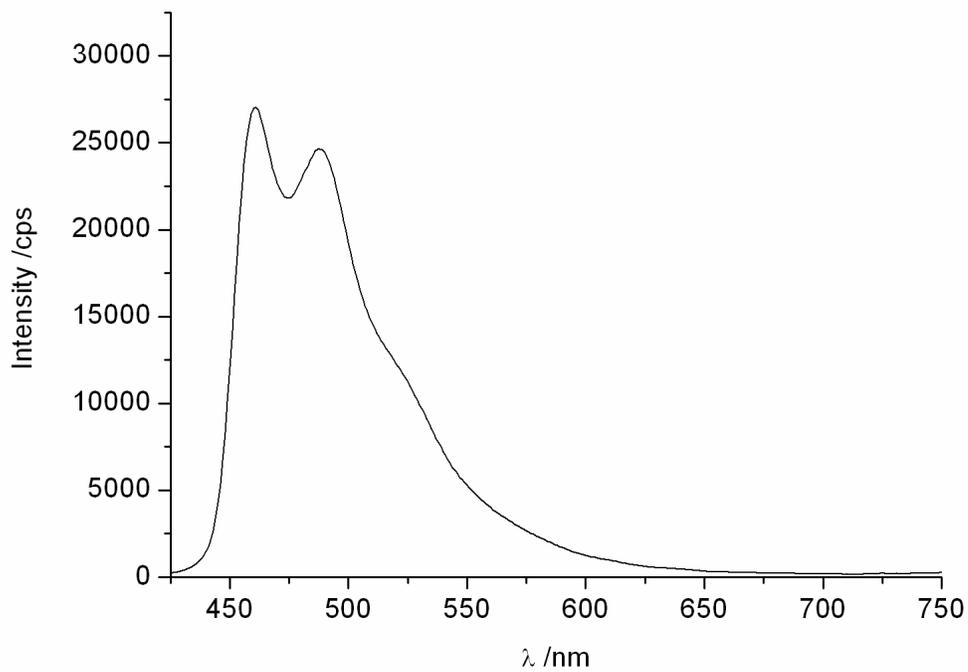
<sup>19</sup>F NMR in CD<sub>3</sub>OD:  $\sigma$  = -108.96 (F pos. 3 with respect to iridium centre); -110.28 (F pos. 3 with respect to iridium centre); -111.21 (F pos. 5 with respect to iridium centre); -112.32 ppm (F pos. 5 with respect to iridium centre).

ESI-MS: Calc: 837.80; experimental 839.13 (protonated species).

FT-IR in KBr: 1685 (C=O stretch); 1604 cm<sup>-1</sup> (C=C stretch).



Absorption spectrum of complex **1**

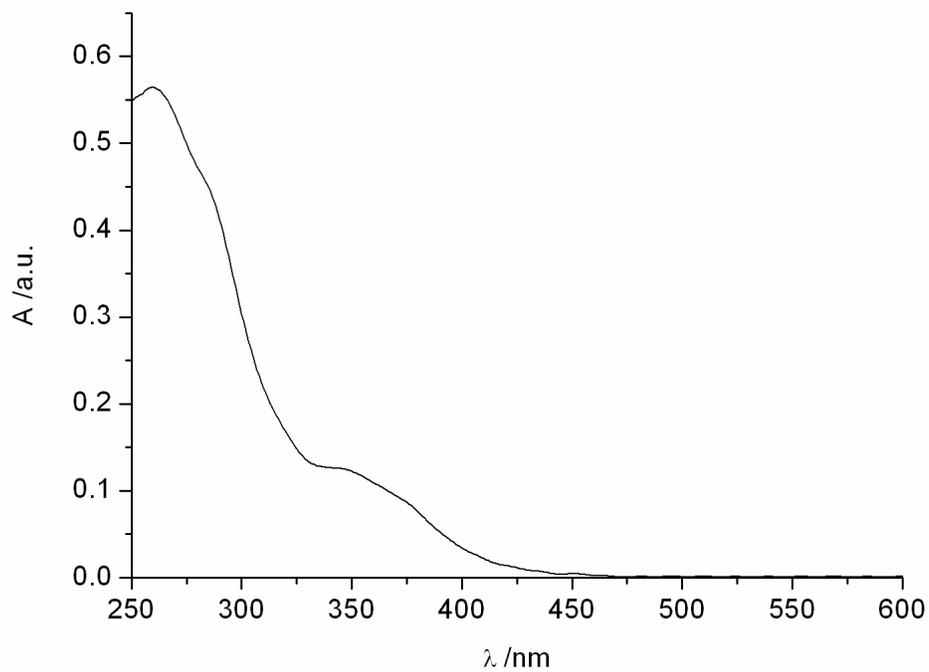


Emission spectrum of complex **1**

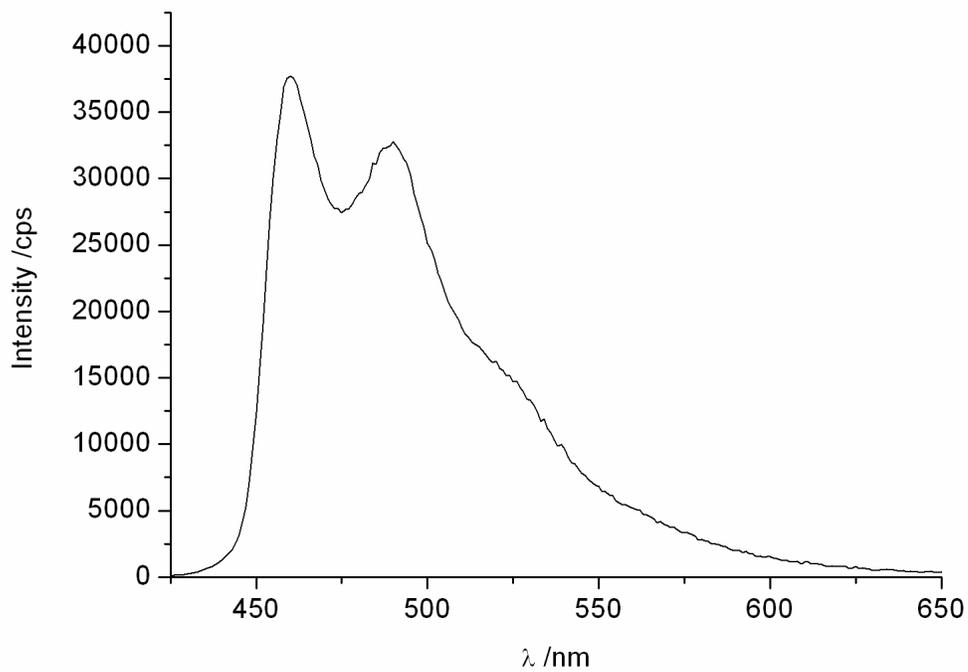
## Complex 1a

Complex **1a** was prepared and purified according to a previously published procedure.<sup>5</sup>

<sup>1</sup>H NMR in CDCl<sub>3</sub>: 8.29 (dd, 2H, aromatics, J=8Hz, 2Hz); 8.22 (d, 1H, aromatic, J=8Hz); 8.12 (d, 2H, aromatics, J=8Hz); 7.85 (dd, 1H, aromatic, J=8Hz, 2Hz); 7.83 (d, 1H, aromatic, J=8Hz); 7.68 (m, 3H, aromatics); 7.49 (d, 1H, aromatic, J=8Hz); 7.35 (dd, 2H, aromatics, J=8Hz, 2Hz); 7.26 (d, 1H, aromatic, J=8Hz); 7.14 (dd, 1H, aromatic, J=8Hz, 2Hz); 6.95 (dd, 1H, aromatic, J=8Hz, 2Hz); 6.87 (dd, 1H, aromatic, J=8Hz, 2Hz); 6.50 (dd, 1H, aromatic, J=8Hz, 2Hz); 6.46 (dd, 1H, aromatic, J=8Hz, 2Hz); 5.79 (d, 1H, aromatic, J=8Hz); 5.74 ppm (d, 1H, aromatic, J=8Hz). <sup>19</sup>F NMR in CDCl<sub>3</sub>: -107.19 (F pos. 3 with respect to iridium centre); -107.93 (F pos. 3 with respect to iridium centre); -109.65 (F pos. 5 with respect to iridium centre); -110.41 ppm (F pos. 5 with respect to iridium centre). <sup>13</sup>C NMR in CDCl<sub>3</sub>: 164.37 (C); 157.80 (C); 156.65 (C); 150.42 (C); 150.39 (C); 150.11 (CH); 149.81 (CH); 146.06 (C); 140.41 (CH); 138.80 (CH); 138.62 (CH); 131.21 (CH); 129.01 (CH); 127.62 (CH); 127.49 (CH); 126.49 (CH); 125.29 (C); 123.53 (CH); 122.85 (CH); 115.26 (C); 114.06 ppm (CH). ESI-MS: found 795.13 protonated species (calc. 793.82). FT-IR in KBr: 1604 (C=C stretch); 1561; 1478; 1410; 1338 cm<sup>-1</sup>.



Absorption spectrum of complex **1a**



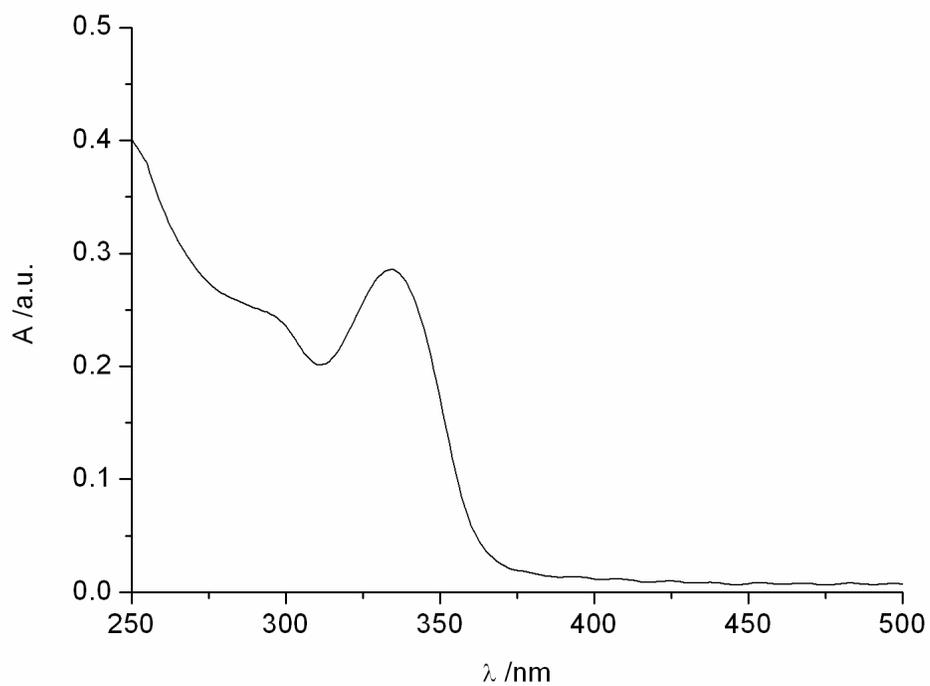
Emission spectrum of complex **1a**

## Complex 2

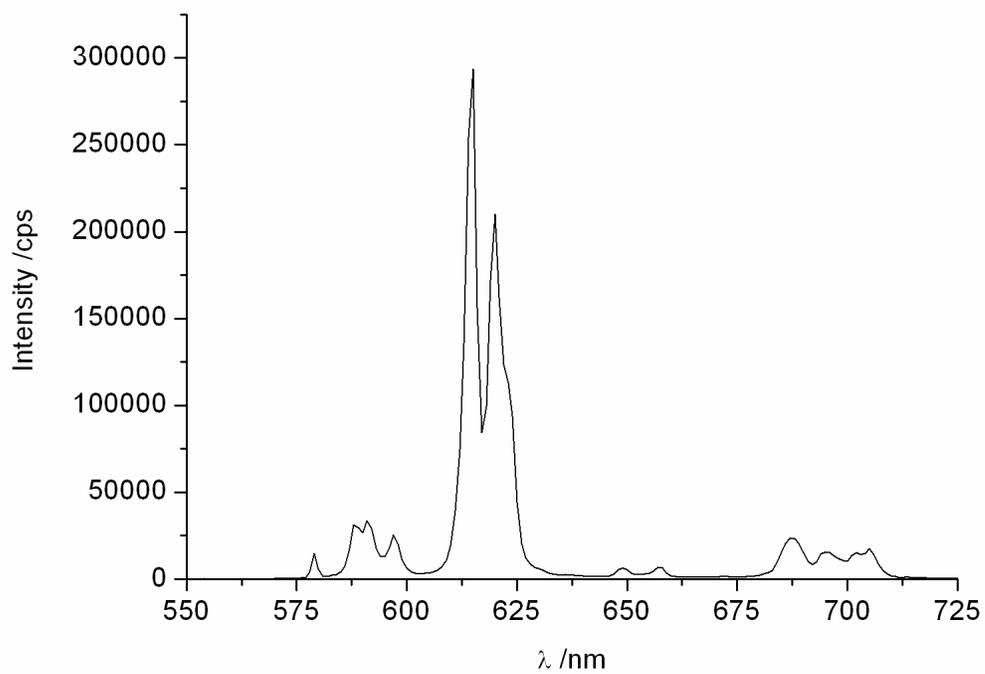
Complex **2** was prepared and purified according to a previously published procedure.<sup>7</sup>

ESI-MS: (calc. 858.93) found 858.93.

FT-IR in KBr (of the MeOH coordinated species): 3380 (OH); 1626; 1565; 1432  $\text{cm}^{-1}$  (C=O stretch).



Absorption spectrum of complex **2**

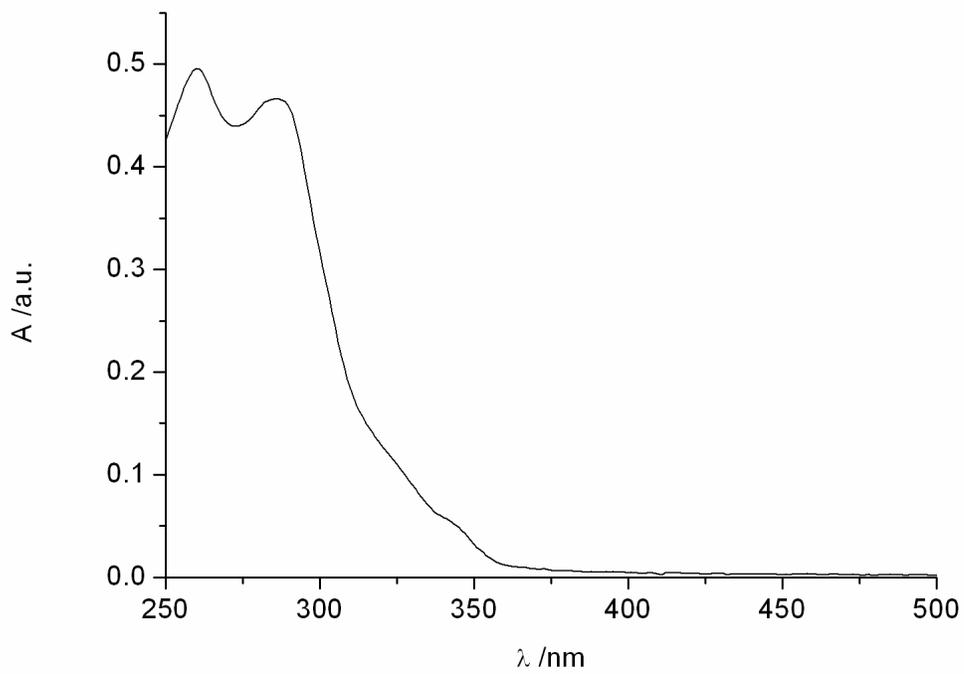


Emission spectrum of complex **2**

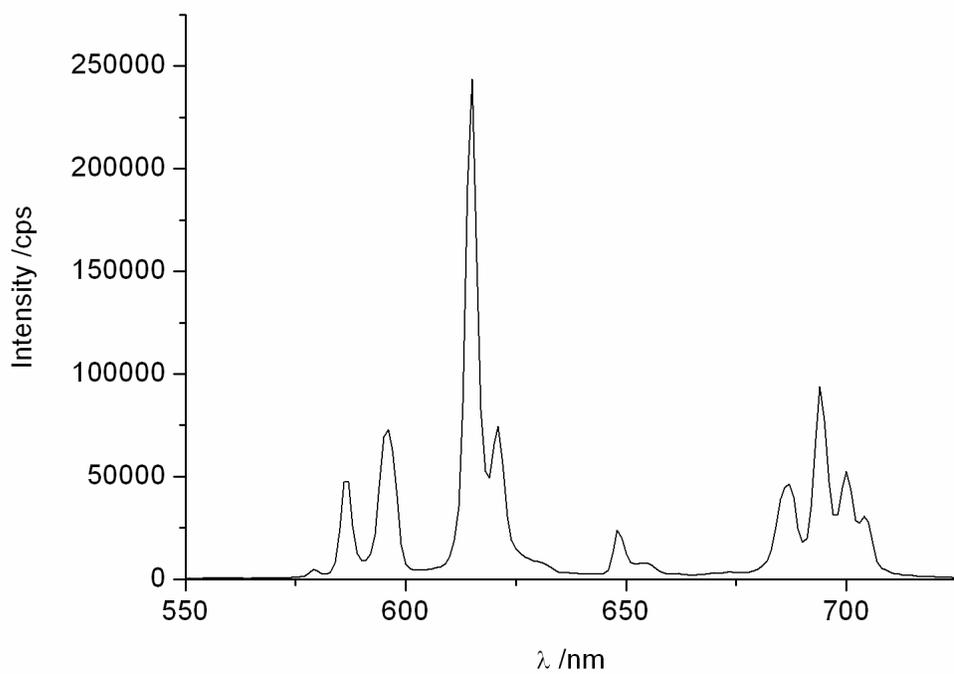
## Complex 2a

Complex **2a** was prepared according to the procedure published by Mukkala et al.<sup>8</sup> The reaction step involving the use of cyanide ions was performed under a gentle stream of nitrogen in a -20°C bath. The exhaust gas was allowed to bubble into a basic solution of NaClO, to oxidise the HCN developed in the reaction vessel.

Spectroscopic data of complex **2a** were consistent with those reported by Mukkala et al.<sup>8</sup>



Absorption spectrum of complex **2a**

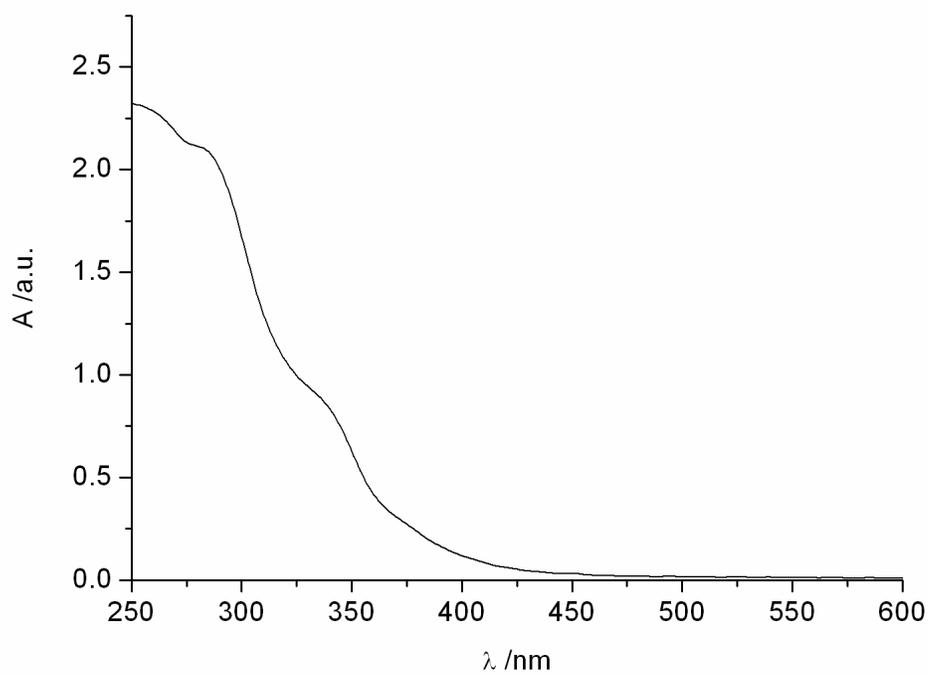


Emission spectrum of complex **2a**

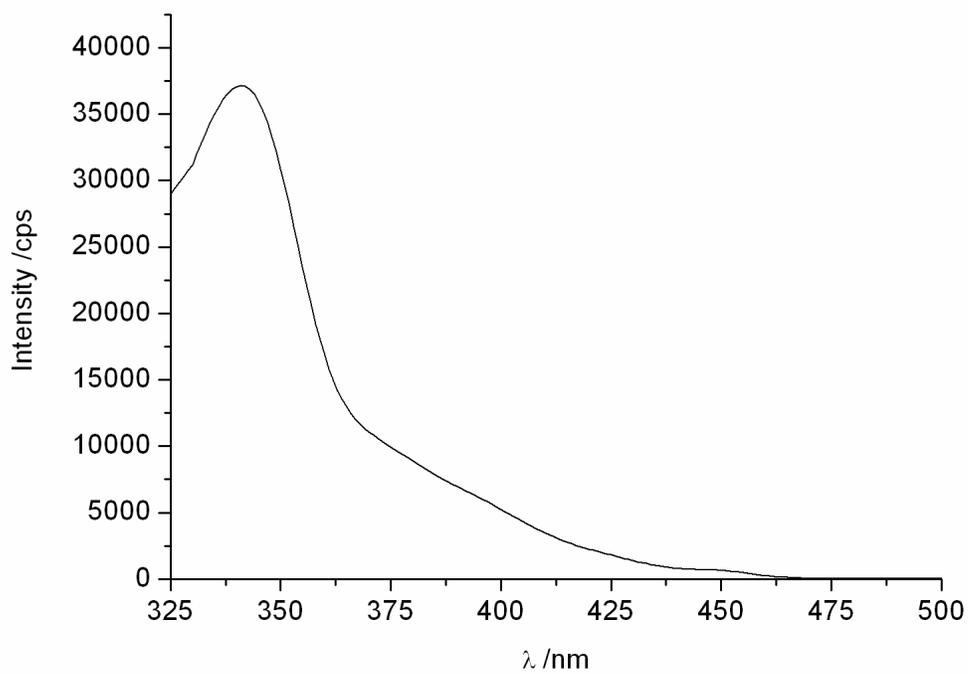
### Complex 3

Complex **1** (30 mg,  $3.5 \times 10^{-5}$  mol) was solubilized in 10 ml of methanol. Complex **2** (15 mg,  $1.75 \times 10^{-5}$  mol) was added portionwise. The mixture was stirred at reflux for 4 hours. The light yellow solution was cooled to room temperature and the solvent was evaporated under reduced pressure. The yellow powder was washed with abundant water and dried under vacuum, to give complex **3** as light yellow amorphous powder (45 mg, 75%).

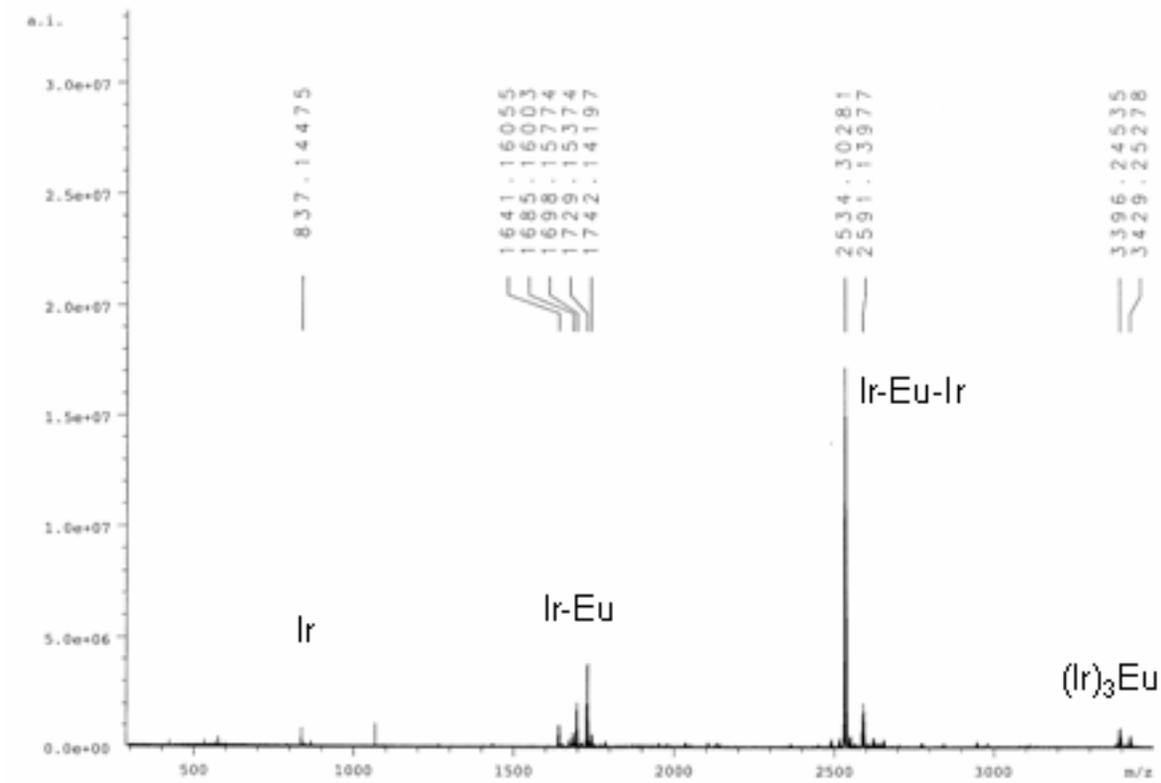
FT-IR in KBr: 1608 (C=C stretch); 1574; 1409  $\text{cm}^{-1}$  (C=O stretch).



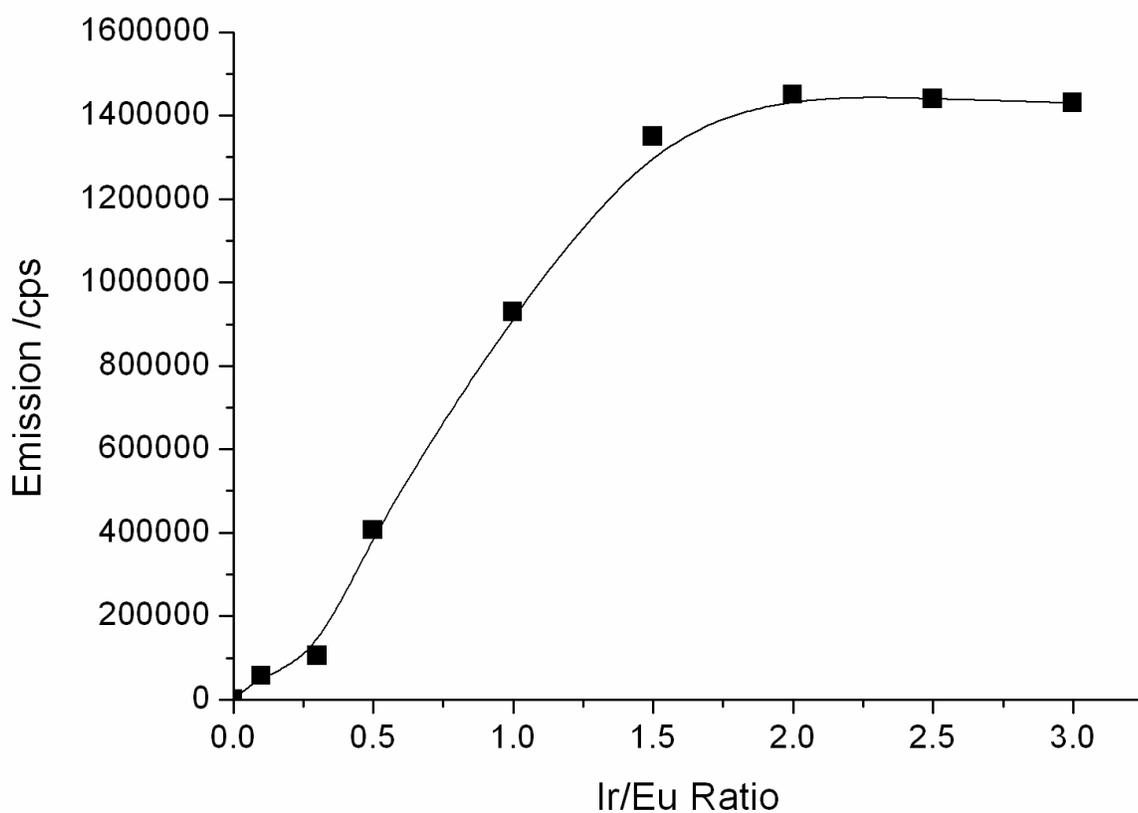
Absorption spectrum of complex **3**



Excitation spectrum of complex **3** (detection at 615 nm).



ESI-mass spectrum of complex **3**, showing the presence of **3** as main product and the 1:1 Ir-Eu adduct as by product. Traces of **1** and of the (Ir)<sub>3</sub>-Eu adduct are also present.



Titration curve of Eu(III) complex **2** against Ir(III) complex **1**. Europium emission upon excitation of Ir(III) at 400 nm, suggest 2:1 composition of Ir(III)-Eu(III) as the most effective.