Electronic Supplementary Material (ESI) for Dalton Transactions.

Blue-Emitting Bolaamphiphile of Zwitterionic Iridium(III) Complex

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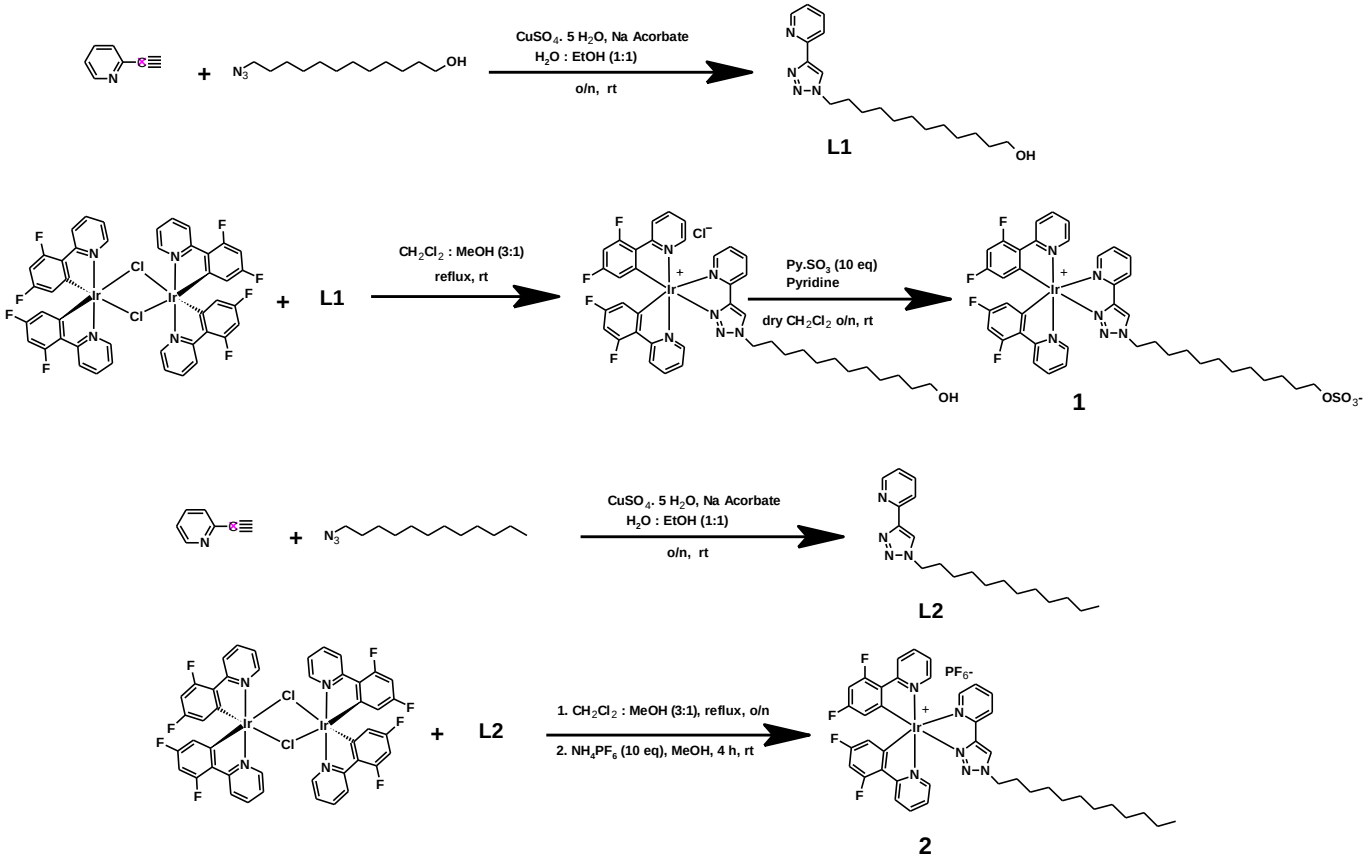
Synthesis Scheme:



X-ray single Crystal Analysis

Complex **1** was crystallized by evaporation in saturated acetonitrile solution, Yellow single crystal of size 0.25 x 0.10 x 0.05 mm were collected

Compound **1** crystallised with two molecules in the asymmetric unit. Both molecules present crystallographically disordered groups (one contains a disordered SO_4 group and the second contains a disordered $[CH_2]_{12}SO_4$ group). Several restraints (SADI, SAME, ISOR and SIMU) were used to improve refinement stability. Additionally, four badly resolved acetonitrile molecules were found in the asymmetric unit and could not be satisfactorily refined. The program SQUEEZE was therefore used to remove mathematically the effect of the solvent. The quoted formula and derived parameters do not include the squeezed solvent molecules.

The refinement crystal data for **1**: $C_{41}H_{41}F_4IrN_6O_4S$, M_r = 982.06, monoclinic, space group $P_{21/c}$ (No. 14), a = 30.6832(7), b = 17.0543(3), c = 17.4993(2) Å, β = 98.576(2)°, V = 9054.7(3) $Å^3$, D_c = 1.531 g cm^{-3}, μ = 3.061 mm^{-1}, Z = 8, λ = 0.71073 Å, T = 223(2) K, 49495 reflections collected (±h, ±k, ±l), [(sinθ)/λ] = 0.66 $Å^{-1}$, 15576 independent (R_{int} = 0.071), and 11656 observed reflections [I ≥ 2σ(I)], 1227 refined parameters, R = 0.062, wR2 = 0.134. CCDC-1531086 for compound **1** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

In Table 1 selected parameters are collected.

Table S1 *Selected bond length (Å) and angles (°) for bolaamphiphile **1**.*

Bond Distance (Å)	Bond Angles (°)	**1a**		**1b**	
		(Å)	(°)	(Å)	(°)
Ir−N11	N21−Ir−N11	2.1702	76.19	2.1589	75.99
Ir−N21	N21−Ir−N41	2.1257	89.29	2.1207	91.12
Ir−N41	N21−Ir−N61	2.0404	95.30	2.0406	94.35
Ir−N61	N21−Ir−C52	2.0493	99.37	2.0549	101.74
Ir−C52	N21−Ir−C72	2.0102	171.83	2.0182	170.23
Ir−C72	N11−Ir−C52	2.0123	173.85	2.0081	175.48
	N41−Ir−N61		173.37		172.12
	N41−Ir−C52		79.62		79.75
	N61−Ir−C72		81.27		82.34
	C521−Ir−C72		88.34		87.67

Figure S1 shows interactions between two dfppy moieties with inverse orientation through a C-F•••π (average distance 3.29 Å) and a C-H••π (average distance 3.22 Å) non-covalent bond

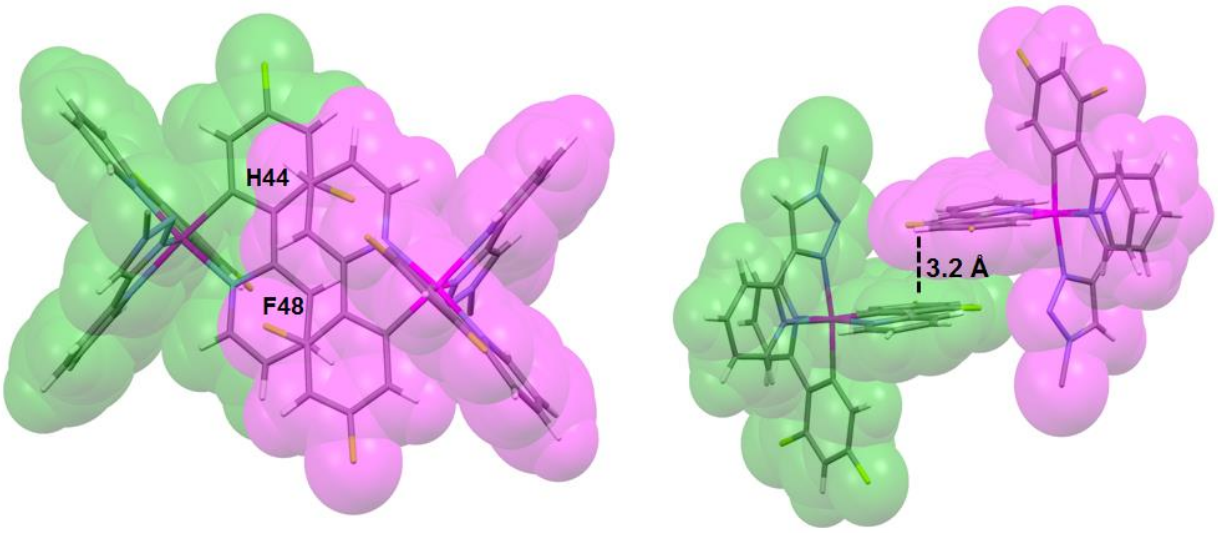


Figure S1. *Head-to-head intermolecular interactions between two molecules of complex* ***1****.*

The same compound display an interesting head-to-tail interaction between the sulphate group and the C-H moieties of the pyridine triazole ligand coordinated to the Ir ion

Figure S3 shows the 4 molecules of complex1 kept in a head tail interaction with sulphate group by the electrostatic CH-O interactions ranged between 2.34 and 2.66 Å

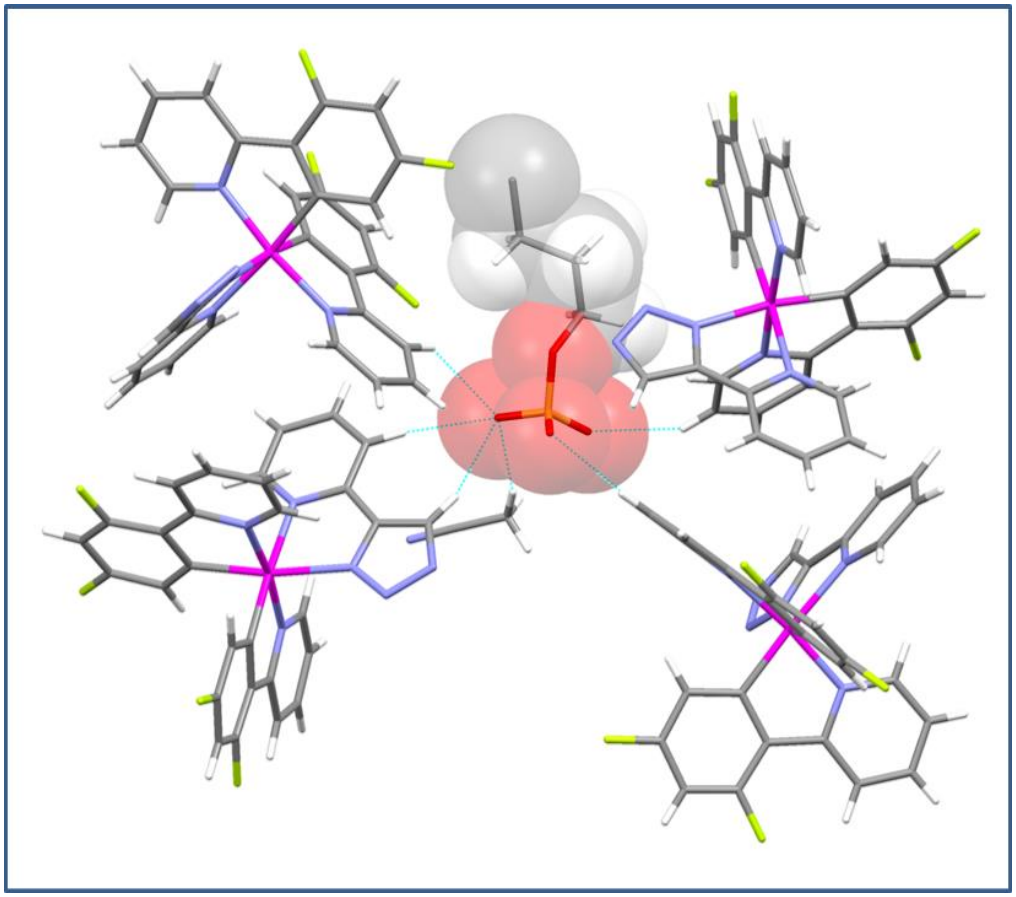


Figure S2 *head-to-tail intermolecular interactions in the packing of complex* ***1****.*

The molecule **1** packs along the b axis with two slightly different orientation that are depicted in Fig S3

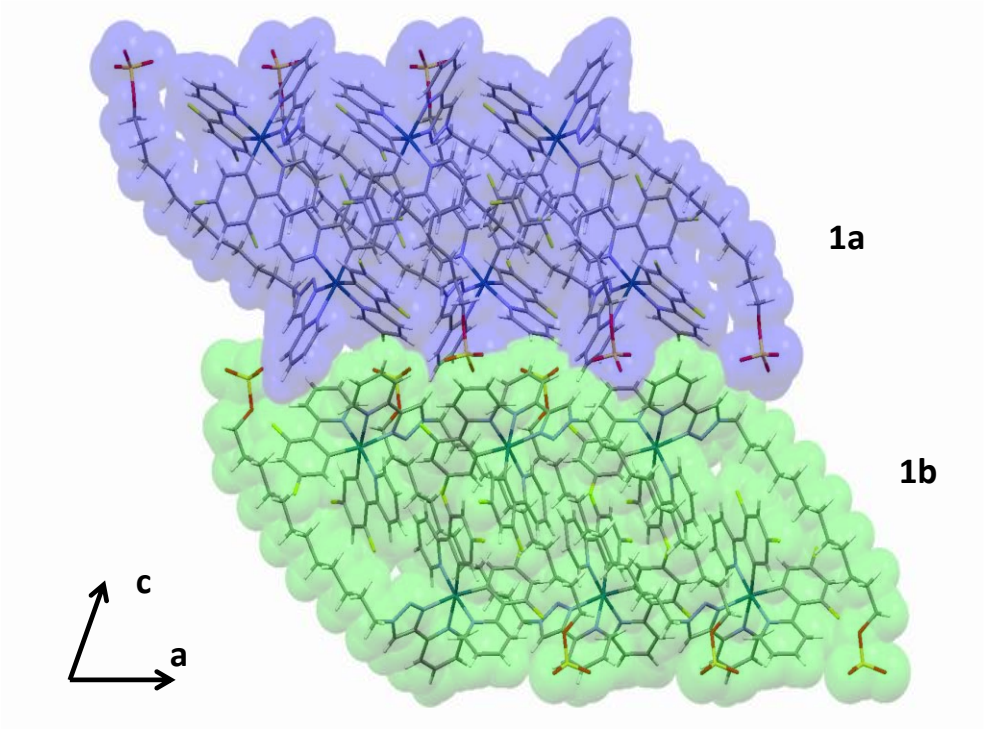


Figure S3. *Crystalline packing of complex **1** along the b-axis*

Low temperature (77 K) emission spectra of **1** and **2**, where recorded in rigid matrix of butryonitirile

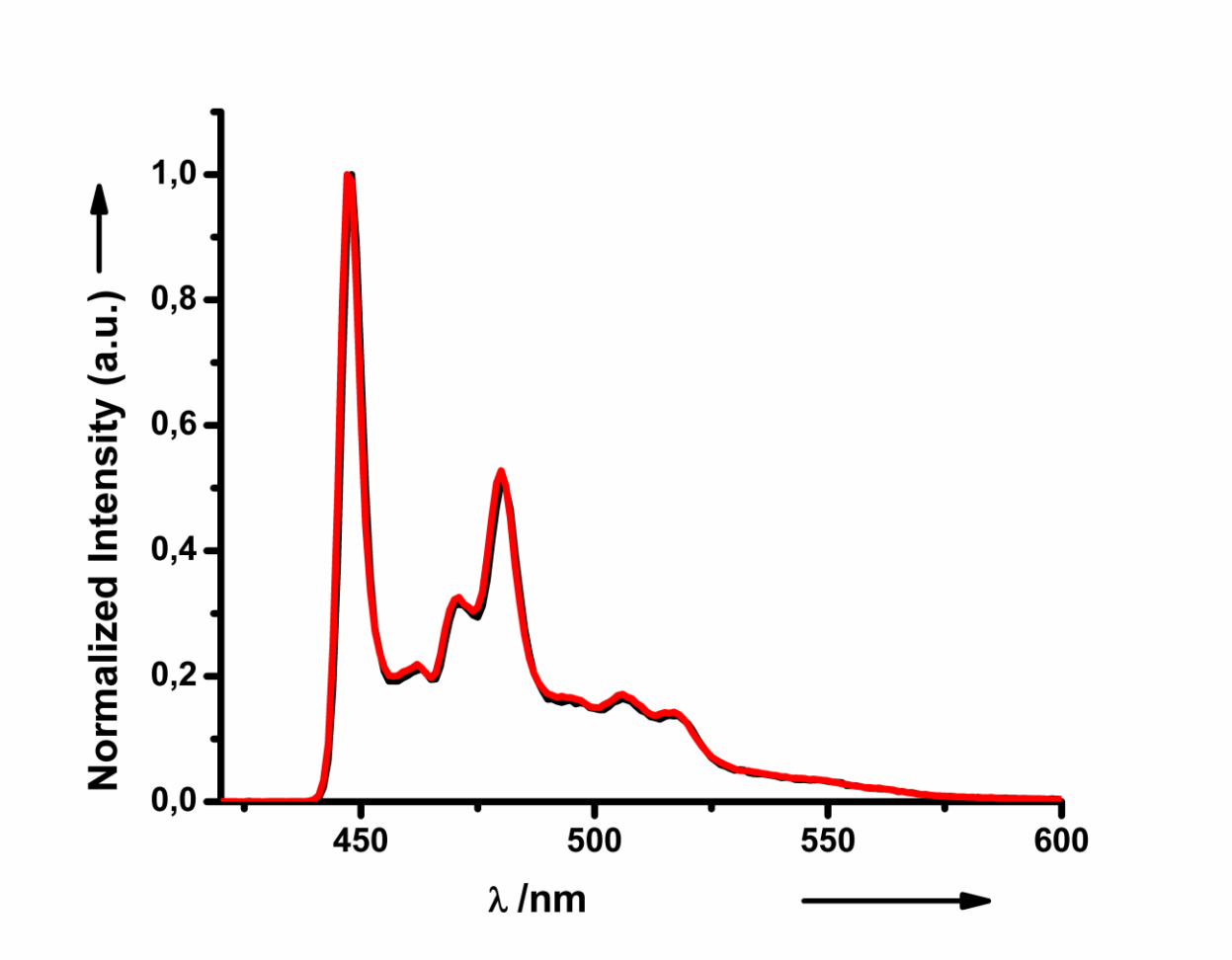


Figure S4. *Emission of **1** and **2** at 77 K (butyronitrile)*

***Electrochemistry**. CV plots recorded in acetonitrile solutions (concentration = 10^{-4}M) of complexes **1** and **2** using TBAF as electrolyte (0.1M) are displayed in Figure S5*

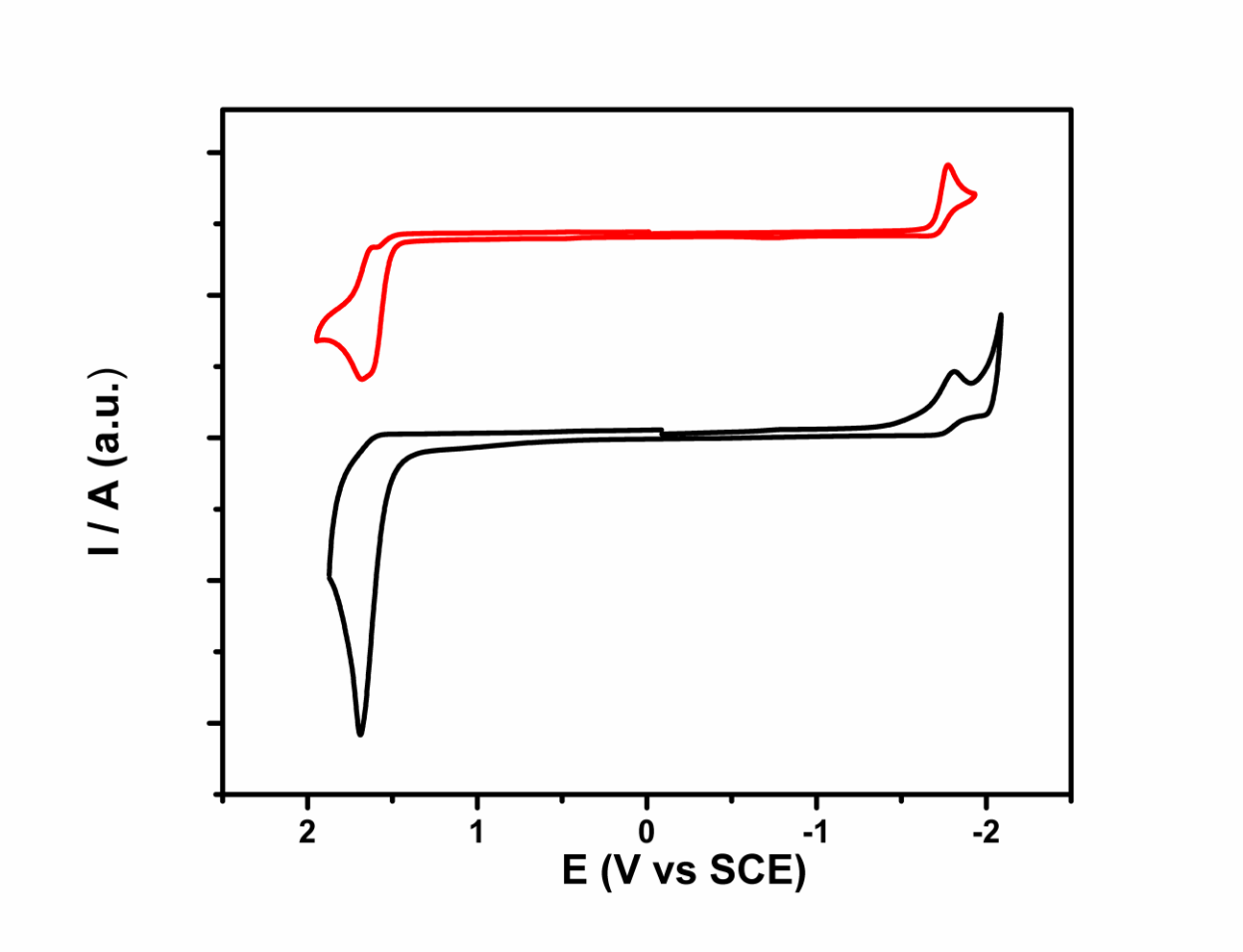


***Figure S5** Cyclic voltammetry curves of the compounds **1** (black) and **2** (red) with Fc/Fc+ as reference and set as zero, in a solution 0.1 M of TBAH in acetonitrile*

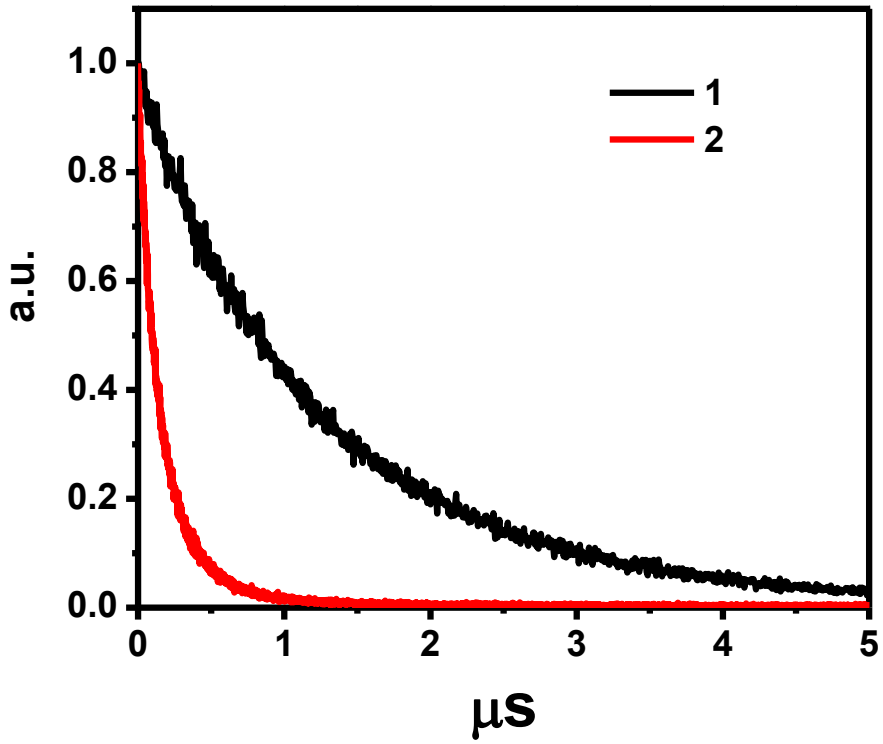


Figure S6 Excited state *decay curves for* ***1 (black)*** *and* ***2*** *(red) in solid states at room temperature.*

λ_{exc} *=365 nm*