Supporting Information

Alkoxy-substituted difluoroboron benzoylmethanes for photonics applications: a photophysical and spectroscopic study

María José Mayoral,[a] Paloma Ovejero,[a] Mercedes Cano*[a] and Guillermo Orellana*[b]

[a] *Department of Inorganic Chemistry I, Faculty of Chemistry, Universidad Complutense de Madrid, E-28040 Madrid, Spain. Fax: 34 9139 44352; Tel: 34 91 394 43 41; E-mail: mmcano@quim.ucm.es*
[b] *Department of Organic Chemistry, Faculty of Chemistry, Universidad Complutense de Madrid, E-28040 Madrid, Spain. Fax: 34 9139 44103; Tel: 34 91 394 4220; E-mail: orellana@quim.ucm.es*

Table S1. Fluorescence lifetimes (τ) in ns of adduct **7** as a function of the Reichardt's spectroscopic solvent polarity scale ($E_T^N(30)$)

Solvent	$E_T^N(30)$[a]	τ[b]
Methanol	0.762	1.79
Acetonitrile	0.460	1.75
Acetone	0.355	1.76
Dichloromethane	0.309	1.67
Tetrahydrofuran	0.207	1.73
Toluene	0.099	1.65

[a] C. Reichardt, Solvents and Solvent effects in Organic Chemistry, Wiley-VCH, 2003, pp. 418-425; [b] Uncertainty: ± 3%.

Table S2. Yields and analytical data of the BDFs

	MOLECULAR FORMULA	Yield (%)	Elemental analysis			
			Requires (%)		Found (%)	
			C	H	C	H
1	$C_{27}H_{42}BF_2O_3$	61	66,3	8,2	66,0	8,1
2	$C_{29}H_{46}BF_2O_3$	65	67,7	8,6	67,6	8,3
3	$C_{31}H_{50}BF_2O_3$	63	68,8	9,0	68,9	8,8
4	$C_{33}H_{54}BF_2O_3$	62	69,8	9,3	69,9	8,9
5	$C_{35}H_{51}BF_2O_4$	56	71,9	8,8	71,7	8,9
6	$C_{39}H_{59}BF_2O_4$	52	73,1	9,3	73,0	9,0
7	$C_{43}H_{67}BF_2O_4$	54	74,1	9,7	73,8	9,6
8	$C_{47}H_{75}BF_2O_4$	52	75,0	10,0	75,1	9,7
9	$C_{51}H_{83}BF_2O_4$	53	75,7	10,3	75,5	10,0

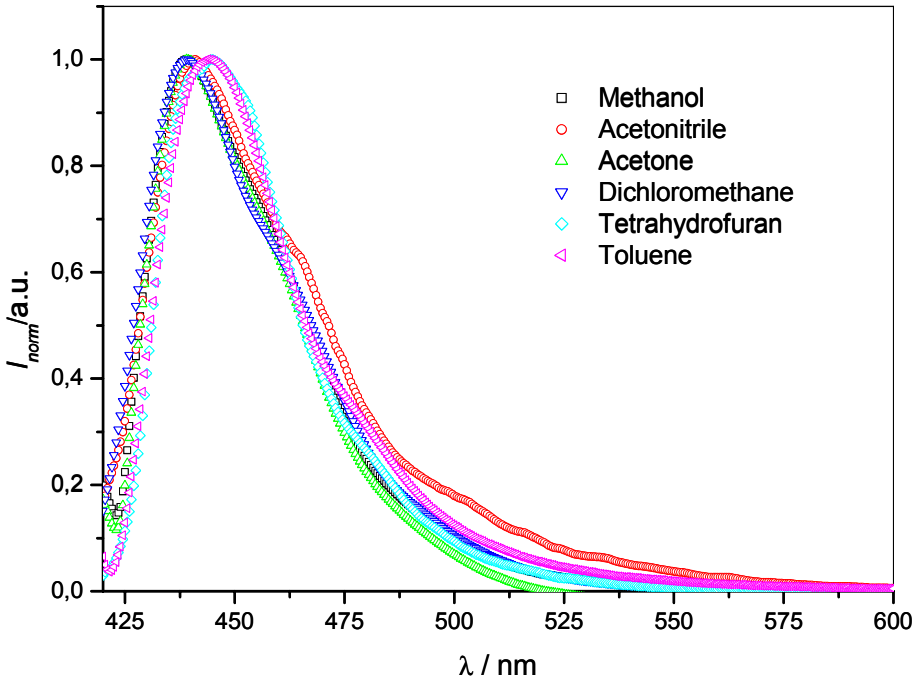

Fig. S1 Normalized fluorescence spectra of adduct **7** (λ_{ex} = 415 nm) in different solvents at room temperature (1-5 x 10^{-5} M)

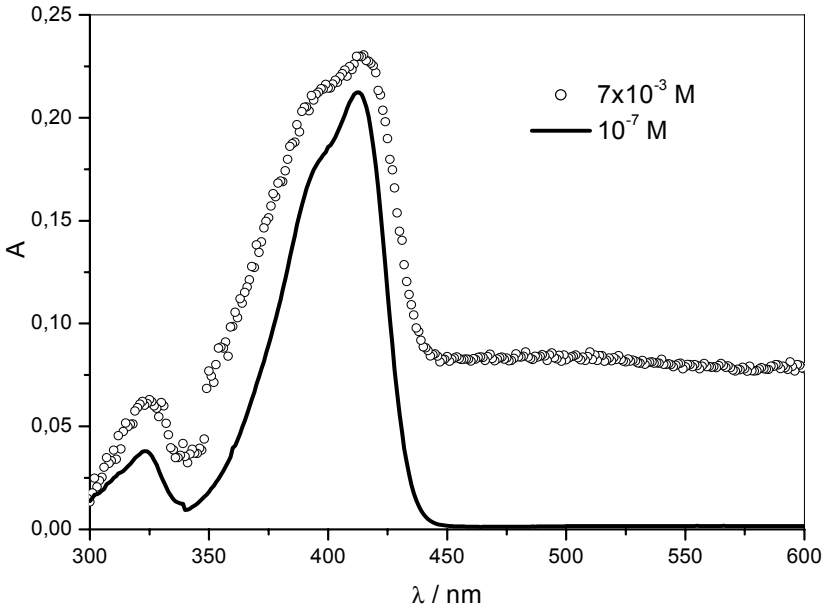

Fig. S2 UV-Vis absorption spectra of adduct **7** of 10^{-7} and 7 x 10^{-3} M solutions in dichloromethane. The latter spectrum was recorded using a 1 mm pathlength Hellma absorption cell in the *front face* configuration on a Cary 5 spectrophotometer fit with the diffuse reflectance accessory.

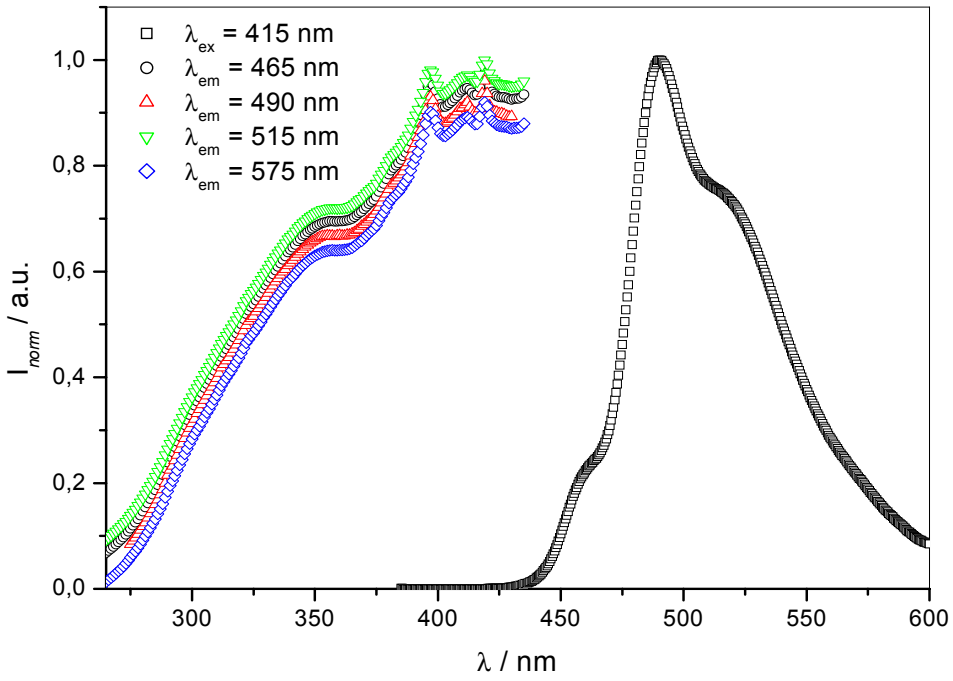

Fig. S3 Normalized excitation and emission spectra of adduct **7** of 7 x 10^{-3} M solutions in dichloromethane acquired in the *front face* configuration. The excitation spectra have been offset for the sake of comparison.

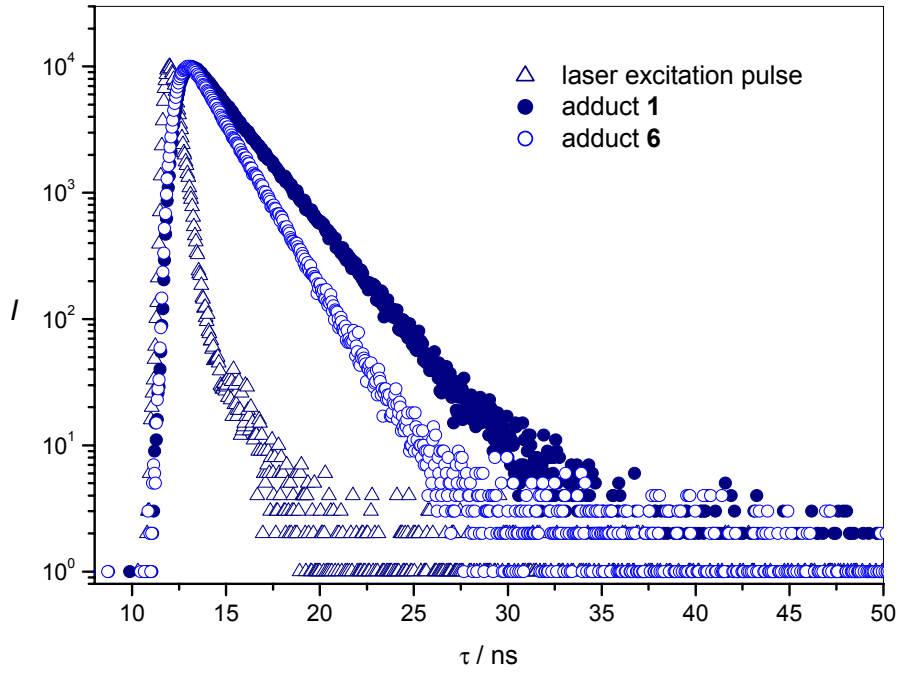

Fig. S4 Diode laser excitation pulse profile (△) and emission decay curves of adducts **1** (τ = 2.32 ns with χ^2 = 1.018) (●) and **6** (τ= 1.68 ns with χ^2 = 1.031)() in 2 x 10^{-7} M dichloromethane solution analyzed as a monoexponential function.

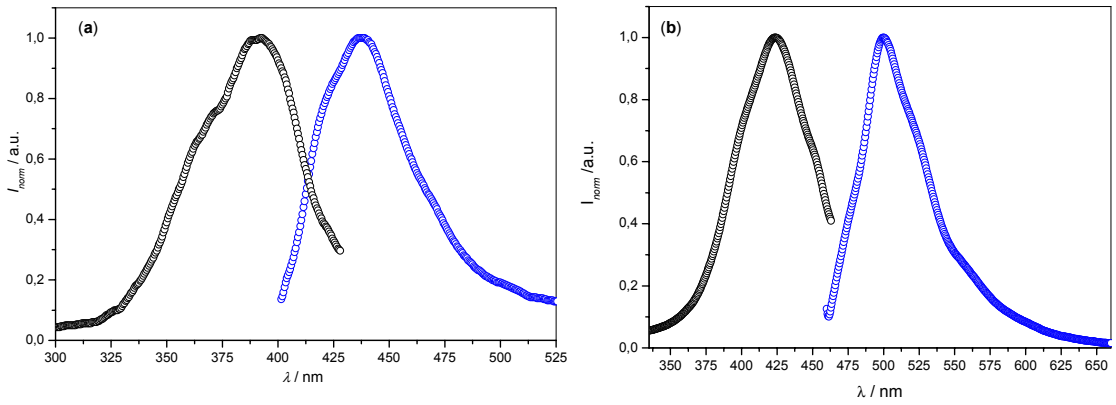

Fig. S5 Normalized excitation and emission spectra of adducts (a) **2** and (b) **9** in the solid state (front face configuration).

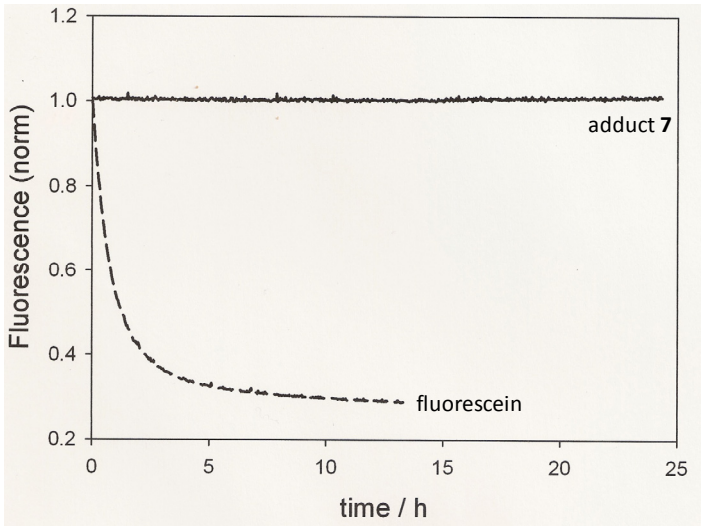

Fig. S6 Comparison of the photostability of fluorescein and **7** in EtOH/H_2O (1:5v/v) under laser light (He-Cd, 442 nm, 5.8 mW). The absorbance at the excitation wavelength was 2.0 in both cases.