Electronic Supplementary Material (ESI) for Dalton Transactions

New Lanthanide-CB[6] Coordination Compounds: Relationships between the Crystal Structure and Luminescent Properties.

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Supporting Information

Hydrogen bond Tables.

Please note that in some cases not all the hydrogen bonds are formed and only the strongest interactions were tabulated. Please be aware that positions of hydrogen atoms are subject of relatively large errors.

Table S1. Hydrogen-bond geometry (Å, °) for **(1)**

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7A···O3	0.82 (2)	2.00 (3)	2.805 (7)	170 (14)
O7—H7B···O14	0.82 (2)	1.89 (2)	2.710 (8)	174 (9)
O8—H8A···Cl3	0.82 (2)	2.40 (3)	3.220 (5)	172 (9)
O8—H8B···O6^{i}	0.82 (2)	1.89 (4)	2.662 (7)	155 (9)
O9—H9A···Cl1^{ii}	0.81 (2)	2.65 (4)	3.409 (7)	156 (8)
O9—H9B···O4^{iii}	0.82 (2)	2.10 (3)	2.918 (8)	171 (9)
O10—H10A···Cl1^{ii}	0.81 (2)	2.23 (2)	3.034 (5)	177 (8)
O10—H10B···Cl2iv	0.80 (2)	2.40 (3)	3.168 (6)	161 (6)
O11—H11A···Cl2iv	0.82 (2)	2.27 (4)	3.045 (6)	156 (8)
O11—H11B···Cl1	0.82 (2)	2.24 (3)	3.025 (5)	160 (7)
O12—H12A···Cl1	0.82 (2)	2.48 (4)	3.238 (7)	155 (7)
O12—H12B···Cl3	0.83 (2)	2.38 (5)	3.174 (6)	161 (11)
O13—H13C···Cl2	0.83 (2)	2.34 (3)	3.149 (8)	164 (10)
O13—H13D···Cl3	0.83 (2)	2.46 (4)	3.257 (8)	160 (8)
O14—H14A···Cl3	0.82 (2)	2.38 (3)	3.190 (5)	168 (9)
O14—H14B···O5^{i}	0.82 (2)	1.99 (2)	2.815 (7)	180 (9)

Symmetry codes: (i) −x, −y, −z; (ii) x, −y+1/2, z+1/2; (iii) −x, y+1/2, −z+1/2; (iv) −x+1, y−1/2, −z+1/2.

Table S2. Hydrogen-bond geometry (Å, °) for **(2)**

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7B···O14	0.83 (2)	1.90 (4)	2.698 (7)	161 (10)
O8—H8A···Cl3	0.83 (2)	2.39 (2)	3.213 (5)	170 (8)
O8—H8B···O6^{i}	0.82 (2)	1.85 (3)	2.648 (6)	165 (9)
O9—H9B···O4^{ii}	0.82 (2)	2.27 (6)	2.952 (7)	141 (9)
O10—H10B···Cl2^{iii}	0.81 (2)	2.36 (2)	3.161 (6)	173 (7)
O11—H11A···Cl2^{iii}	0.82 (2)	2.24 (3)	3.050 (5)	169 (7)
O11—H11B···Cl1	0.82 (2)	2.21 (2)	3.026 (5)	176 (10)
O12—H12A···Cl1	0.82 (2)	2.45 (3)	3.243 (6)	163 (9)
O12—H12B···Cl3	0.83 (2)	2.37 (3)	3.177 (6)	164 (9)
O13—H13C···Cl2	0.83 (2)	2.40 (4)	3.193 (7)	160 (10)
O13—H13D···Cl3	0.83 (2)	2.43 (3)	3.247 (7)	166 (8)
O14—H14A···Cl3	0.82 (2)	2.39 (3)	3.196 (5)	171 (9)
O14—H14B···O5^{i}	0.81 (2)	2.03 (3)	2.811 (6)	162 (9)

Symmetry codes: (i) −x, −y, −z; (ii) −x, y+1/2, −z+1/2; (iii) −x+1, y−1/2, −z+1/2.

Table S3. Hydrogen-bond geometry (Å, °) for **(3)**

D—*H*···*A*	*D*—*H*	*H*···*A*	*D*···*A*	*D*—*H*···*A*
O7—H7B···O14	0.81 (2)	1.87 (2)	2.682 (4)	173 (5)
O8—H8A···Cl3	0.83 (2)	2.40 (2)	3.213 (3)	171 (5)
O8—H8B···O6^{i}	0.82 (2)	1.83 (2)	2.640 (4)	170 (6)
O9—H9B···O4^{ii}	0.82 (2)	2.09 (2)	2.910 (5)	177 (7)
O10—H10B···Cl2^{iii}	0.81 (2)	2.32 (2)	3.128 (3)	174 (5)
O11—H11A···Cl2^{iii}	0.82 (2)	2.24 (2)	3.031 (3)	163 (5)
O11—H11B···Cl1	0.82 (2)	2.22 (3)	2.998 (3)	159 (7)
O12—H12A···Cl1	0.81 (2)	2.42 (3)	3.206 (4)	163 (6)
O12—H12B···Cl3	0.81 (2)	2.40 (4)	3.162 (4)	156 (7)
O13—H13C···Cl2	0.85 (2)	2.28 (2)	3.132 (5)	174 (6)
O13—H13D···Cl3	0.85 (2)	2.38 (3)	3.218 (5)	168 (6)
O14—H14A···Cl3	0.82 (2)	2.36 (2)	3.164 (3)	167 (6)
O14—H14B···O5^{i}	0.81 (2)	2.00 (2)	2.803 (4)	170 (6)

Symmetry codes: (i) −x, −y, −z; (ii) −x, y+1/2, −z+1/2; (iii) −x+1, y−1/2, −z+1/2.

Table S4. Hydrogen-bond geometry (Å, °) for **(4)**

D—*H*···*A*	*D*—*H*	*H*···*A*	*D*···*A*	*D*—*H*···*A*
O7—H7B···O14	0.82 (2)	1.88 (2)	2.692 (6)	170 (5)
O8—H8A···Cl3	0.82 (2)	2.39 (2)	3.207 (4)	176 (7)
O8—H8B···O6^{i}	0.81 (2)	1.84 (2)	2.636 (5)	169 (6)
O9—H9B···O4^{ii}	0.81 (2)	2.10 (3)	2.901 (6)	170 (10)
O10—H10B···Cl2^{iii}	0.81 (2)	2.31 (2)	3.118 (4)	175 (7)
O11—H11A···Cl2^{iii}	0.82 (2)	2.25 (5)	3.027 (5)	158 (10)
O11—H11B···Cl1	0.82 (2)	2.23 (5)	2.993 (4)	155 (9)
O12—H12A···Cl1	0.82 (2)	2.43 (4)	3.213 (5)	160 (8)
O12—H12B···Cl3	0.82 (2)	2.36 (3)	3.167 (5)	167 (7)
O13—H13C···Cl2	0.86 (2)	2.25 (2)	3.101 (8)	173 (7)
O13—H13D···Cl3	0.85 (2)	2.35 (3)	3.198 (8)	172 (7)
O14—H14A···Cl3	0.83 (2)	2.34 (3)	3.152 (4)	166 (7)
O14—H14B···O5^{i}	0.82 (2)	1.97 (2)	2.798 (5)	177 (7)

Symmetry codes: (i) −x, −y, −z; (ii) −x, y+1/2, −z+1/2; (iii) −x+1, y−1/2, −z+1/2.

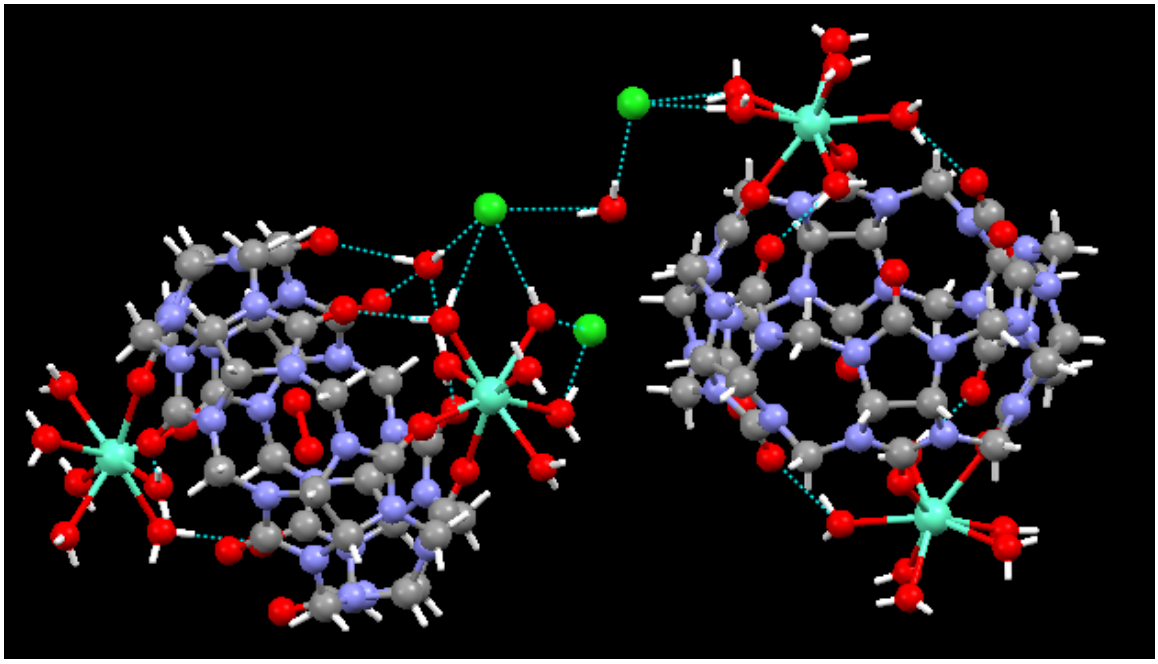

Figure S1. Intermolecular hydrogen bonds in the compound **(1)**.

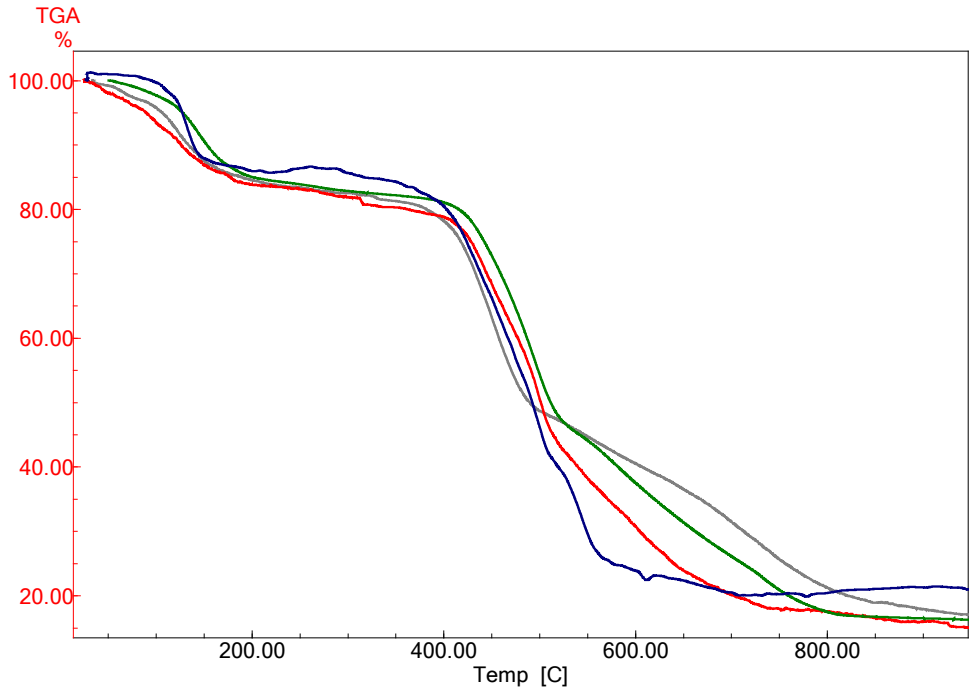

Figure S2. Thermogravimetric analysis of **(1)** (in gray); **(2)** (in red); **(3)** (in green) and **(4)** (in blue).

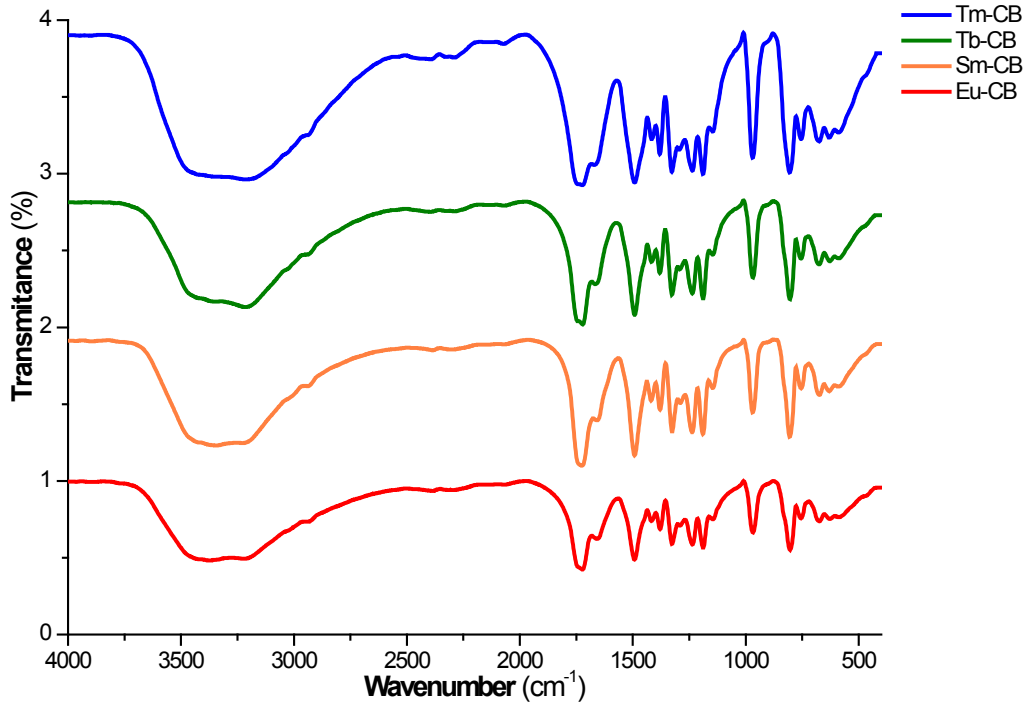

Figure S3. Infrared spectroscopy of the products.

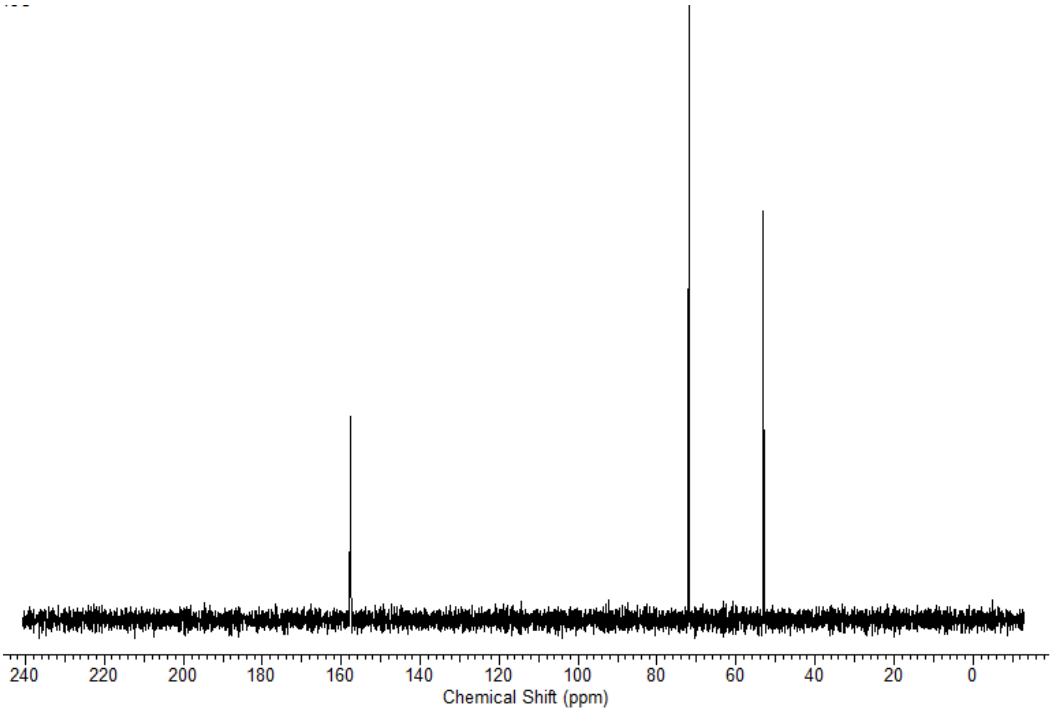

Figure S4. ^{13}C NMR spectrum of the compound **(2)**.

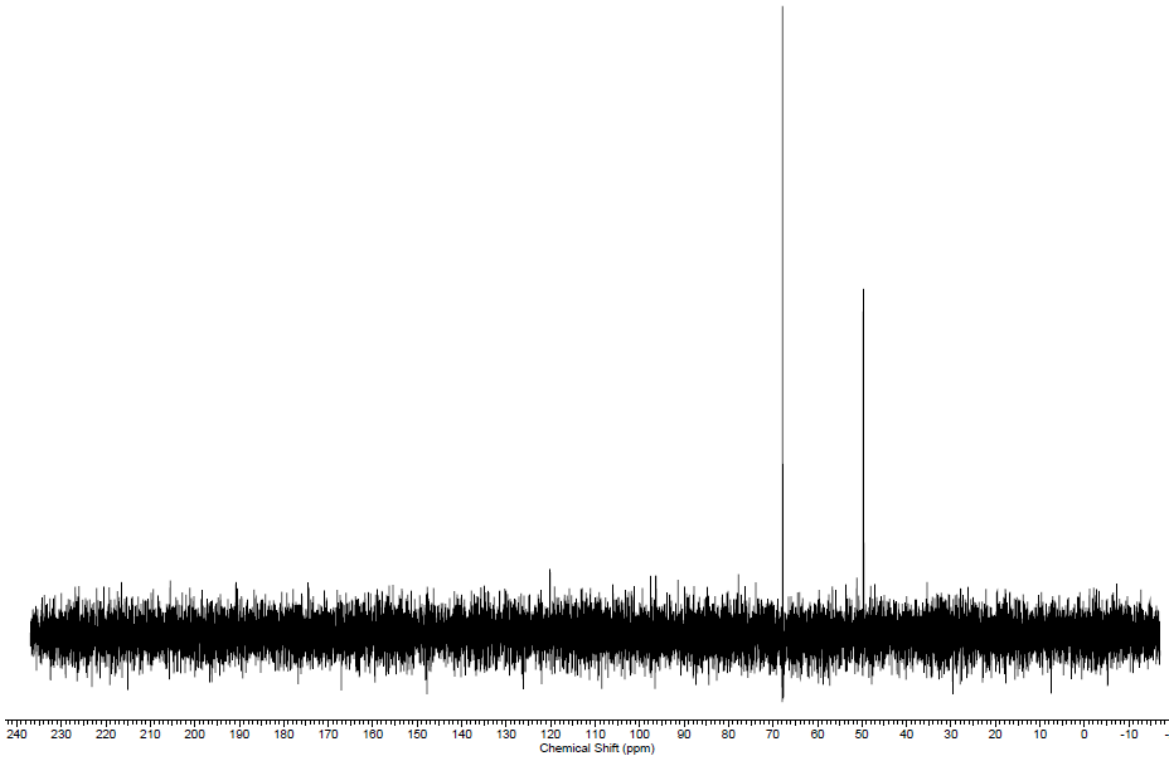

Figure S5. ^{13}C NMR spectrum of the compound **(1)**.

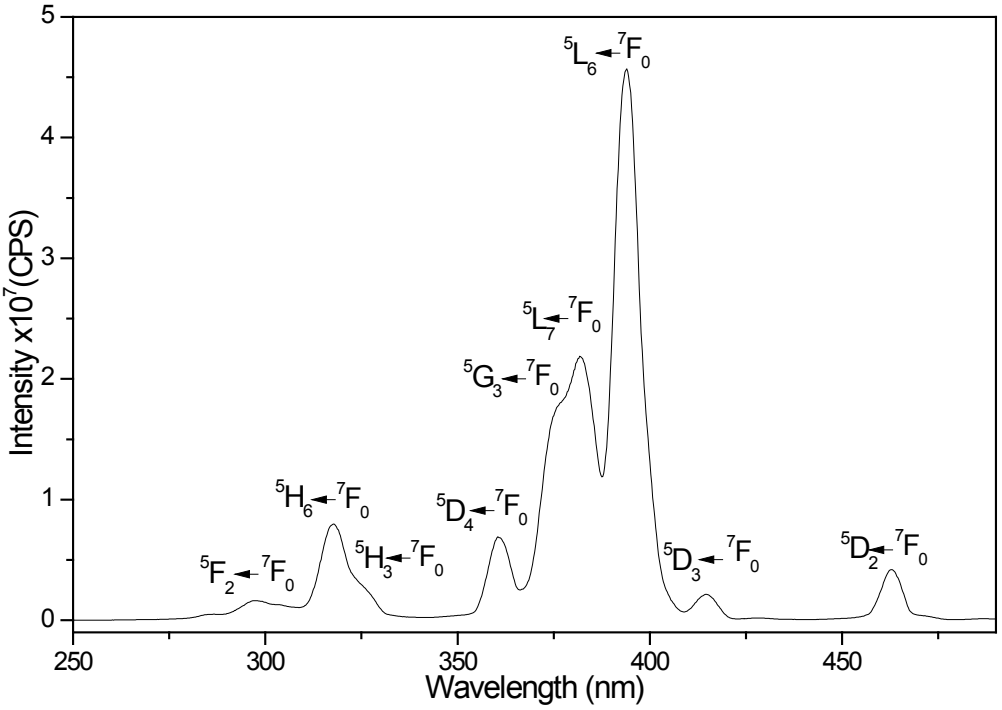

Figure S6. Solid state excitation spectrum of the compound **(1)** monitored in 612 nm at room temperature.

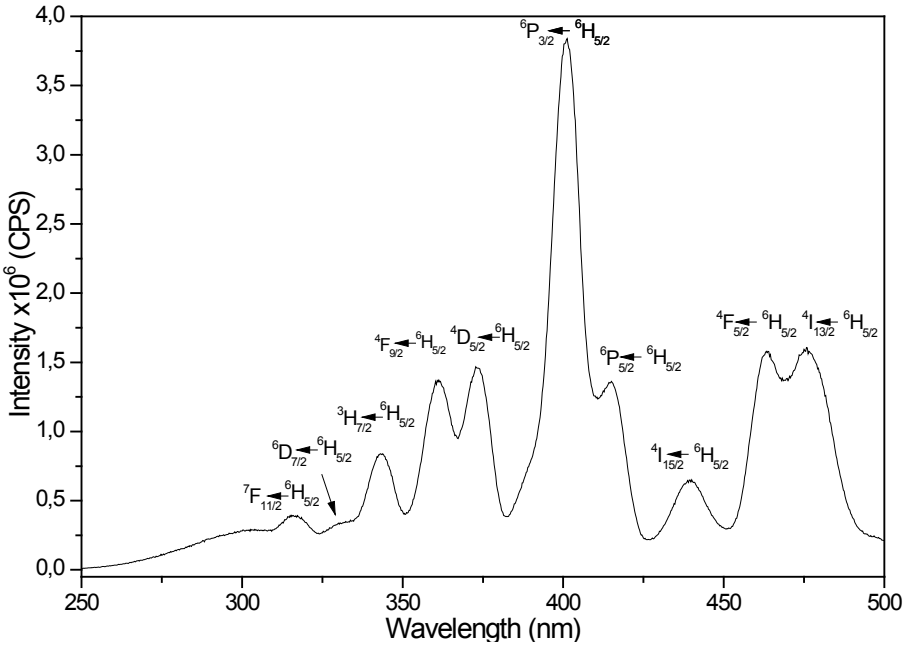

Figure S7. Solid state excitation spectrum of the compound **(2)** monitored in 594 nm at room temperature.

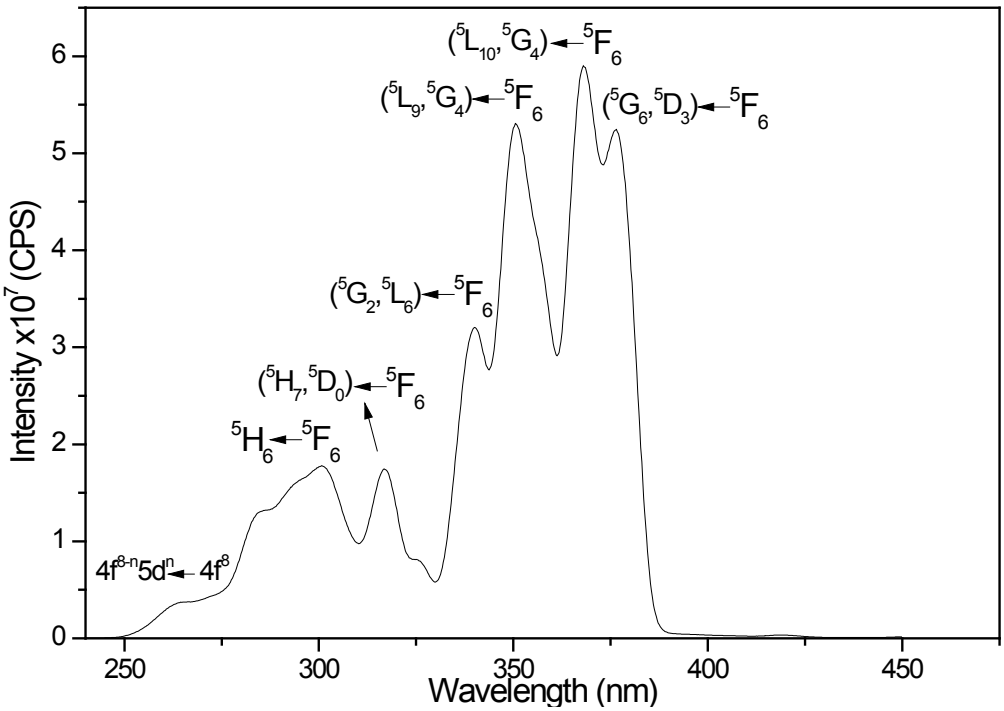

Figure S8. Solid state excitation spectrum of the compound **(3)** monitored in 543 nm at room temperature.

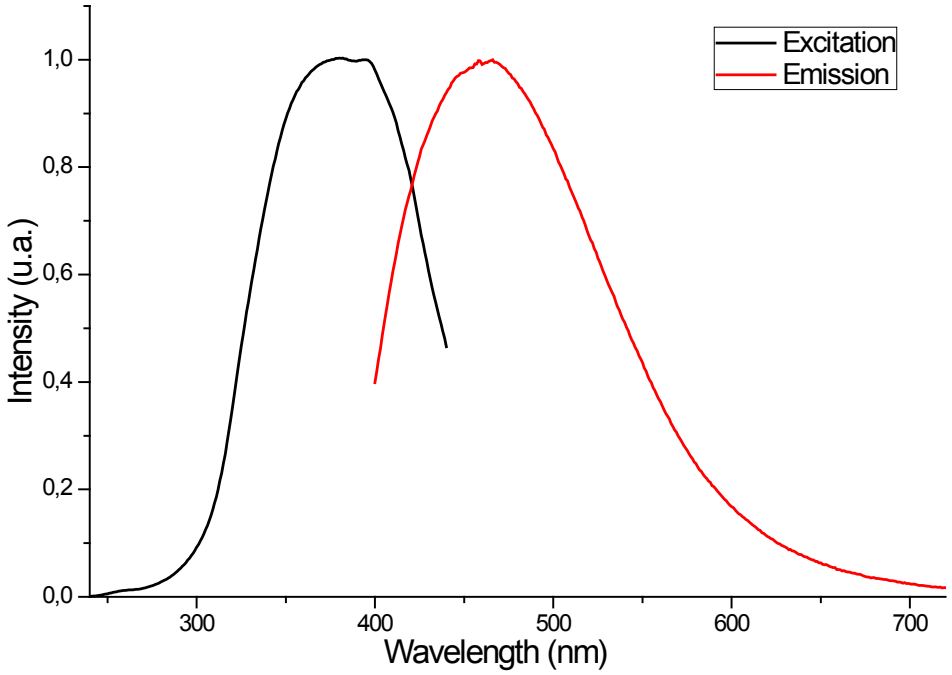

Figure S9. Solid state luminescence spectrum of the free cucurbit[6]uril at room temperature.

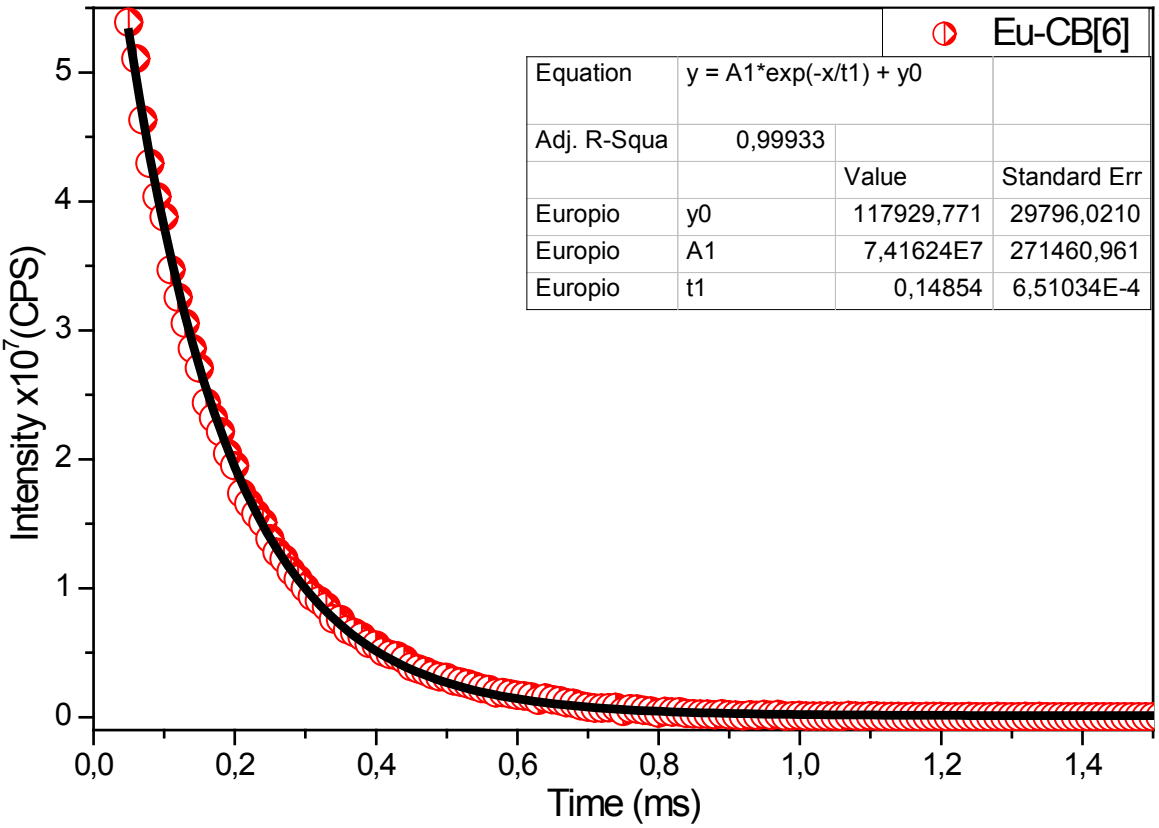

Figure S10. Solid state lifetime decay of **(1)**.

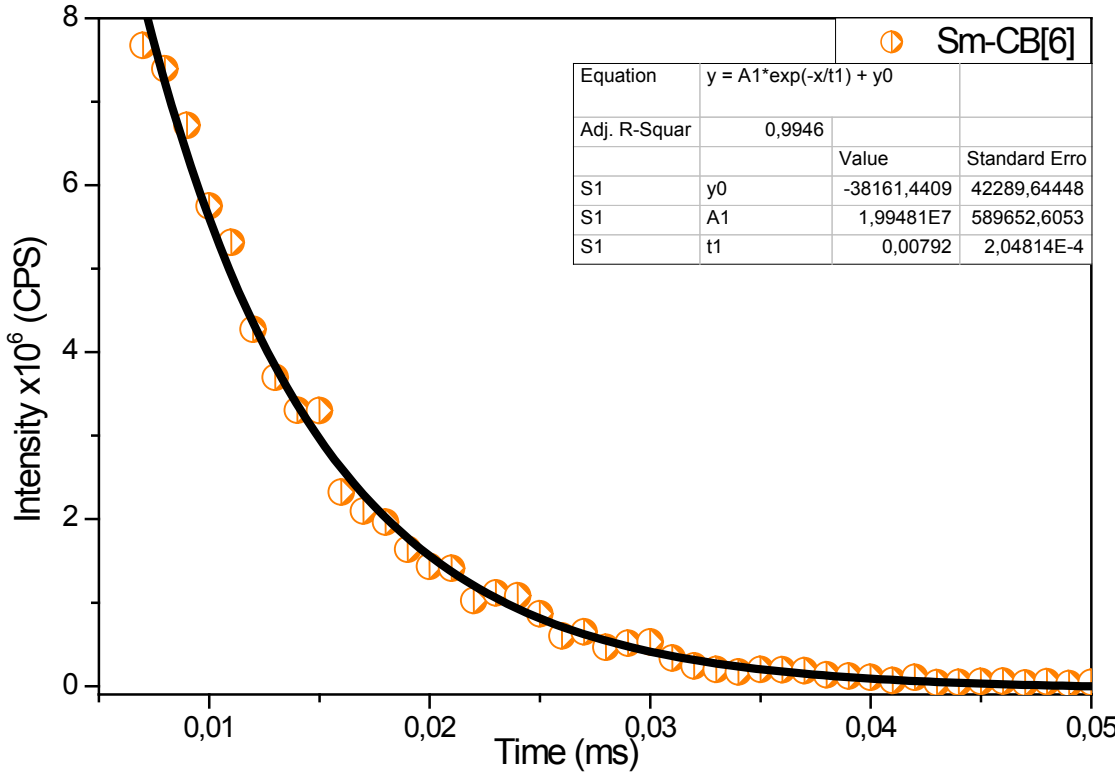

Figure S11. Solid state lifetime decay of **(2)**.

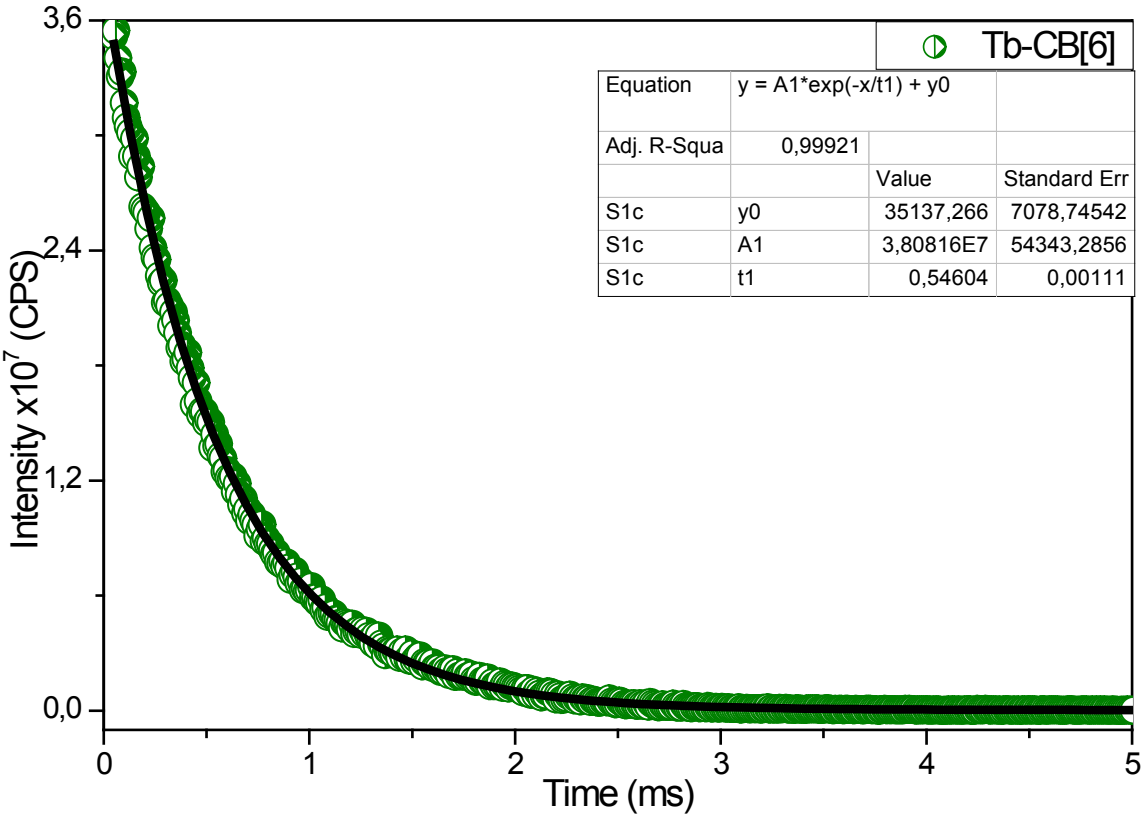

Figure S12. Solid state lifetime decay of **(3)**.

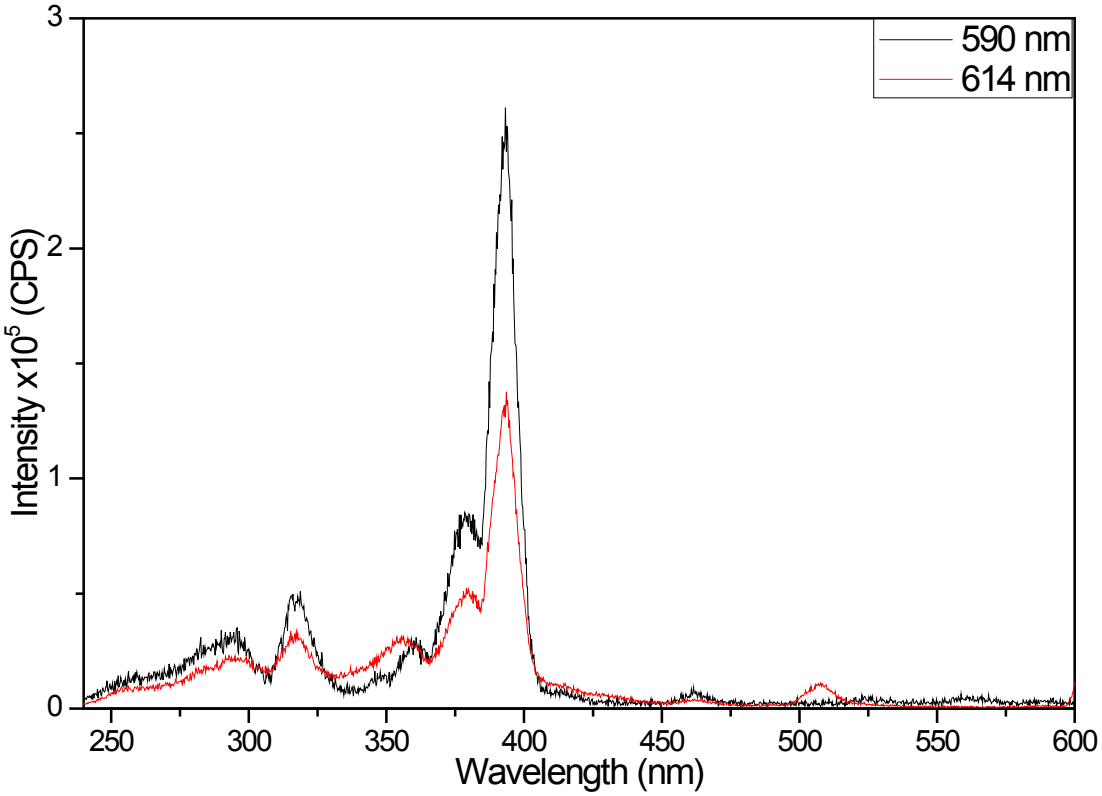

Figure S13. Excitation spectra of **(1)** in aqueous solution.

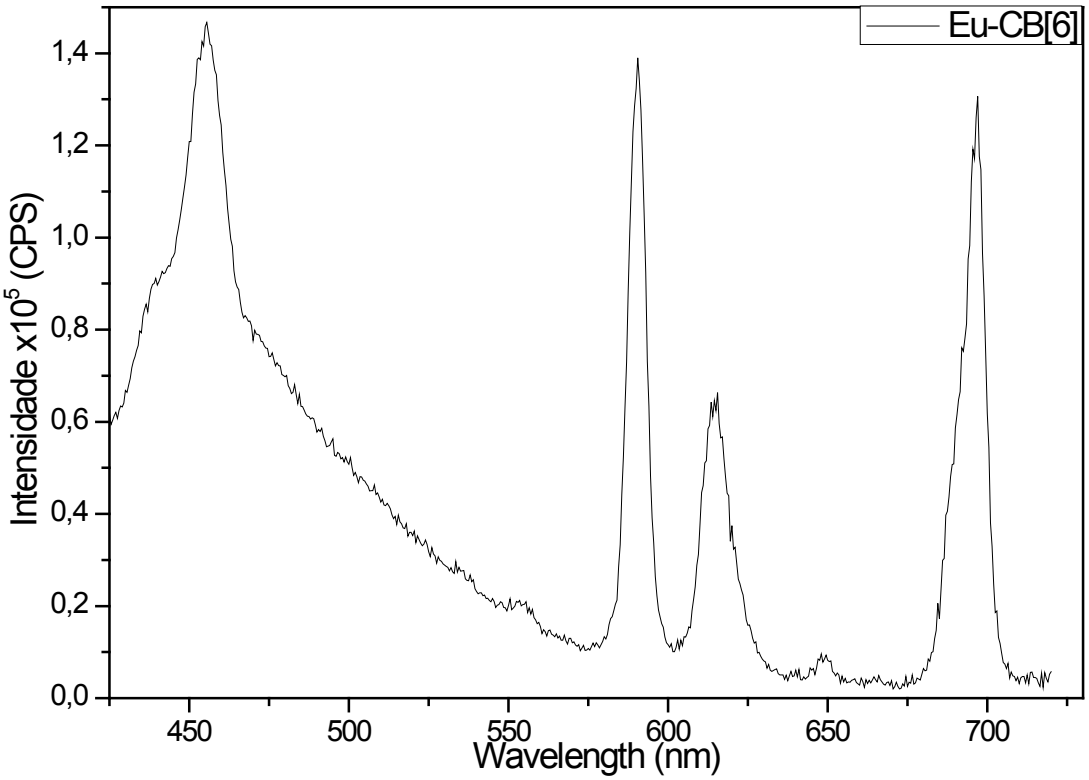

Figure S14. Emission spectrum ($\lambda_{exc.}$ = 395 nm) of **(1)** in aqueous solution.

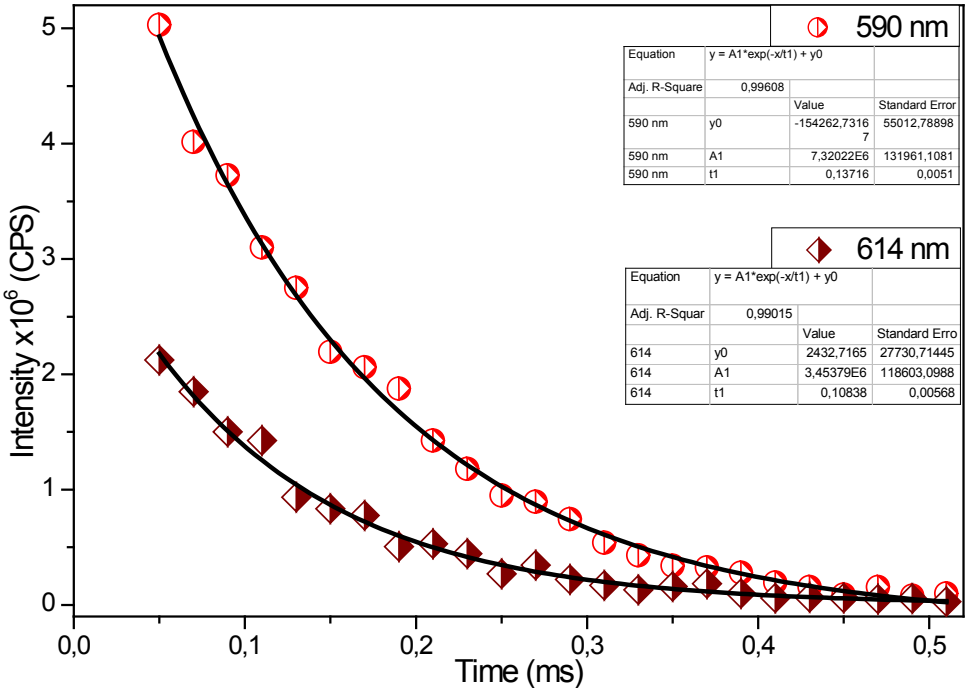

Figure S15. Lifetimes decays **(1)** in aqueous solution.

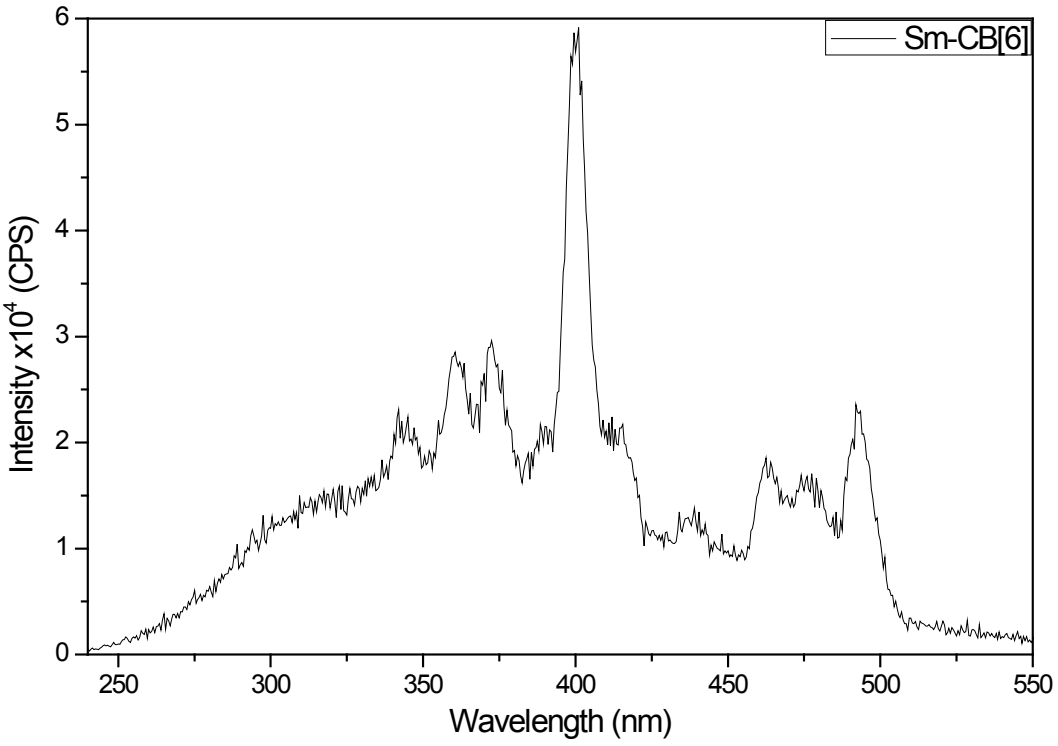

Figure S16. Excitation spectrum ($\lambda_{emis.}$ = 594 nm) of **(2)** in aqueous solution.

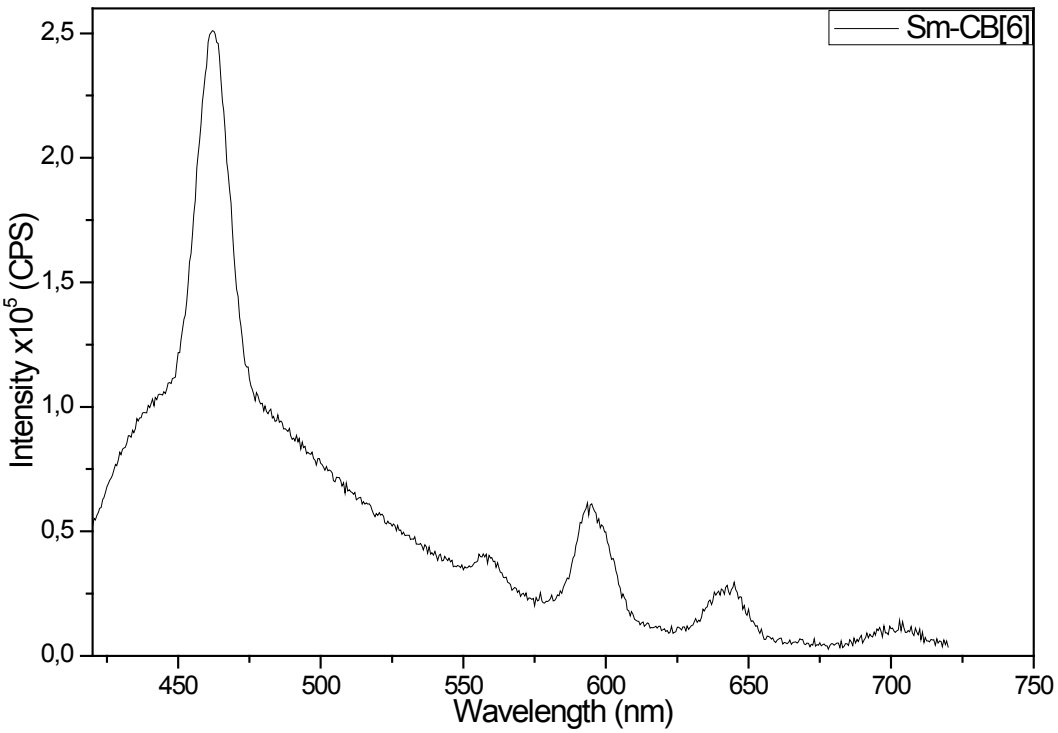

Figure S17. Emission spectrum ($\lambda_{emis.}$ = 400 nm) of **(2)** in aqueous solution.

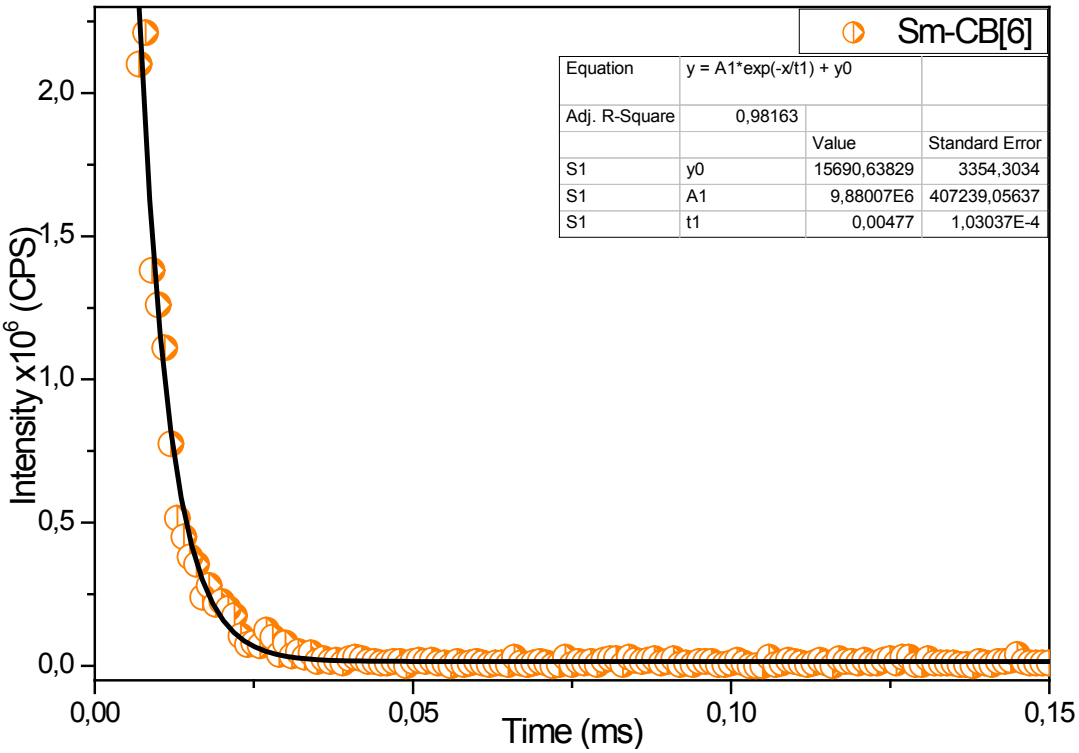

Figure S18. Lifetime decay ($\lambda_{emis.}$ = 594 nm) **(2)** in aqueous solution.

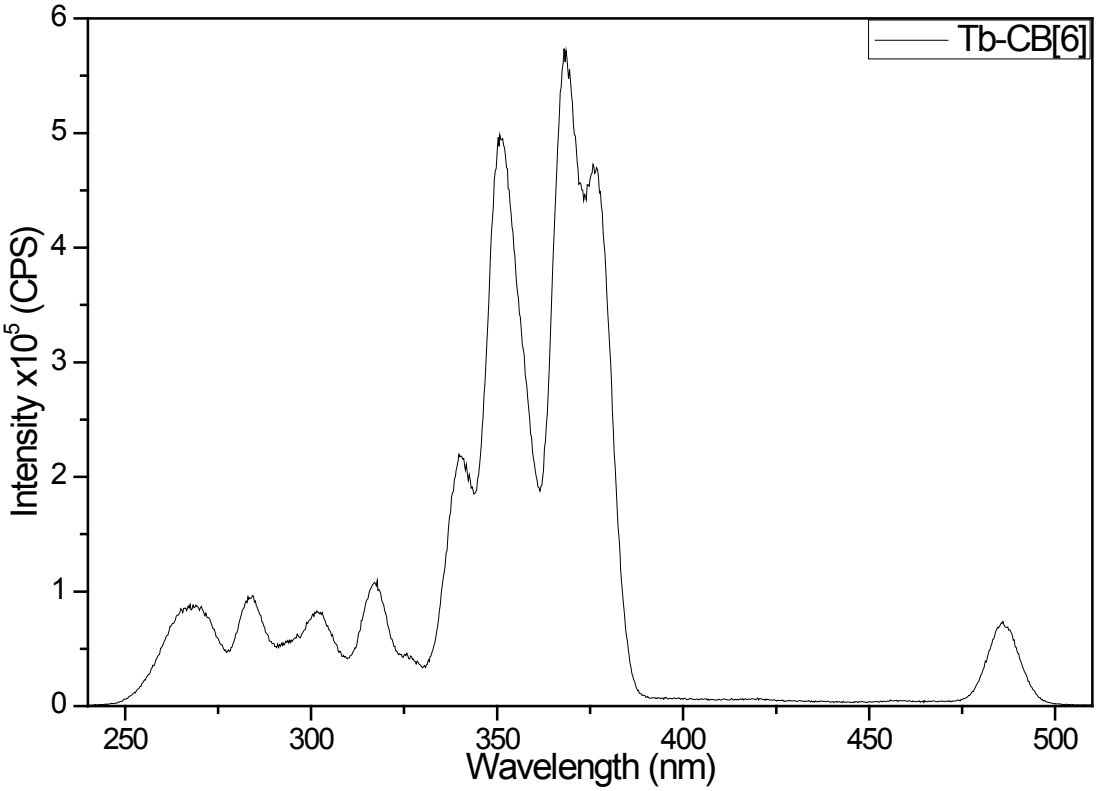

Figure S19. Excitation spectrum ($\lambda_{emis.}$ = 542 nm) of **(3)** in aqueous solution.

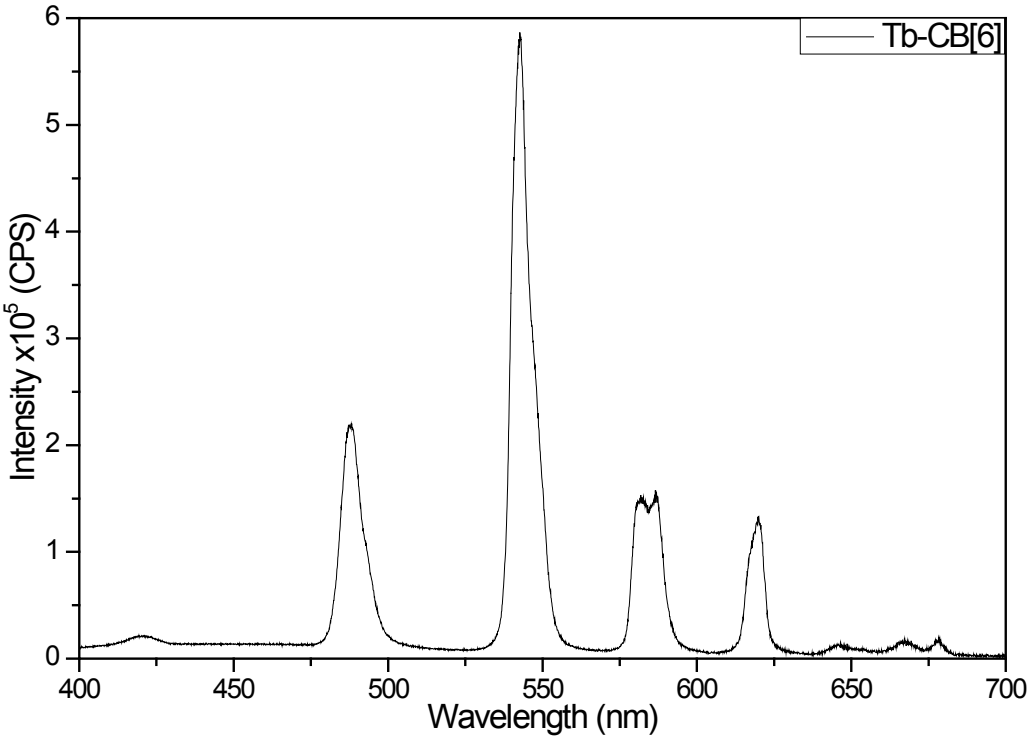

Figure S20. Emission spectrum ($\lambda_{exc.}$ = 368 nm)of **(3)** in aqueous solution.

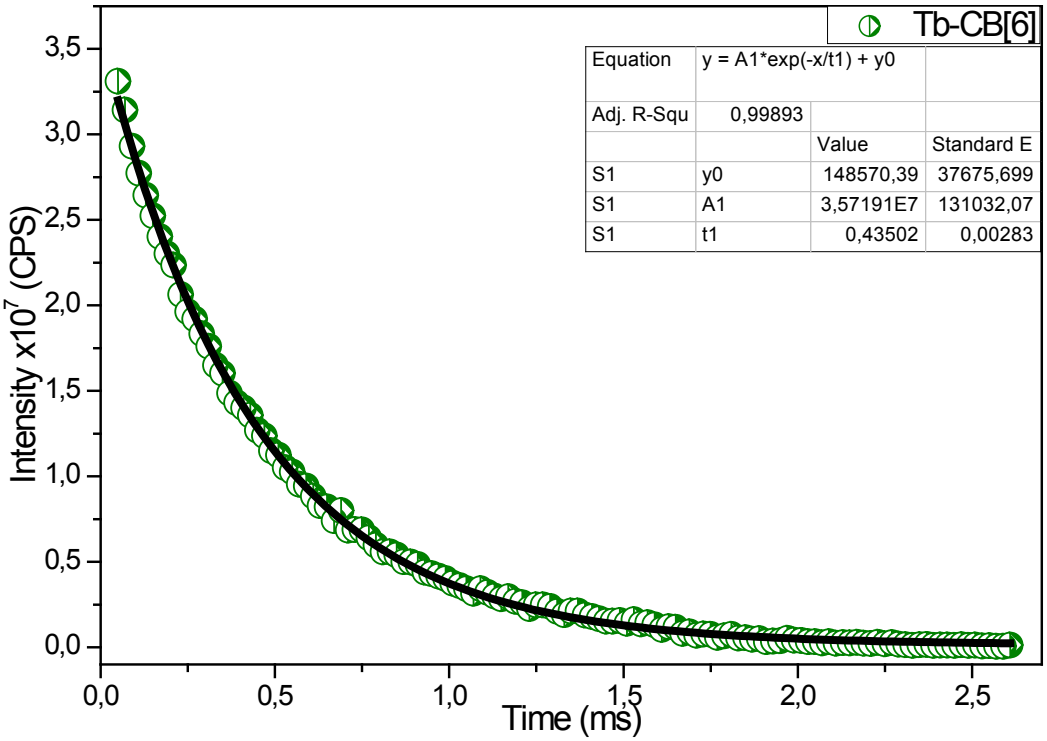

Figure S21. Lifetime ($\lambda_{emis.}$ = 542 nm) **(3)** in aqueous solution.