Electronic Supplementary Material (ESI) for New Journal of Chemistry

Supplementary information (SI)

Bis-silylated terephthalate as a building block precursor for highly fluorescent organic-inorganic hybrid materials

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1. NMR Characterization

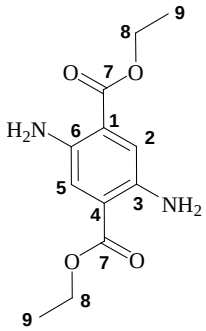

Figure SI1. Description numbers applied to dye **3** to describe de NMR spectra.

Figure SI2. ^{1}H-NMR of the dye **3** in $CDCl_3$.

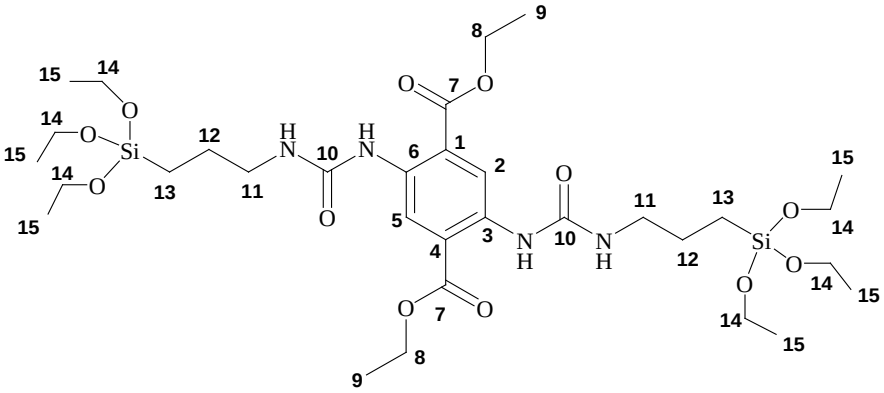

Figure SI3. Description numbers applied to silsesquioxane **5** to describe de NMR spectra.

Figure SI4. ^{1}H-NMR of the silsesquioxane **5** in $CDCl_3$.

Figure SI5. ^{13}C-NMR of the silsesquioxane **5** in DMSO-d^6.

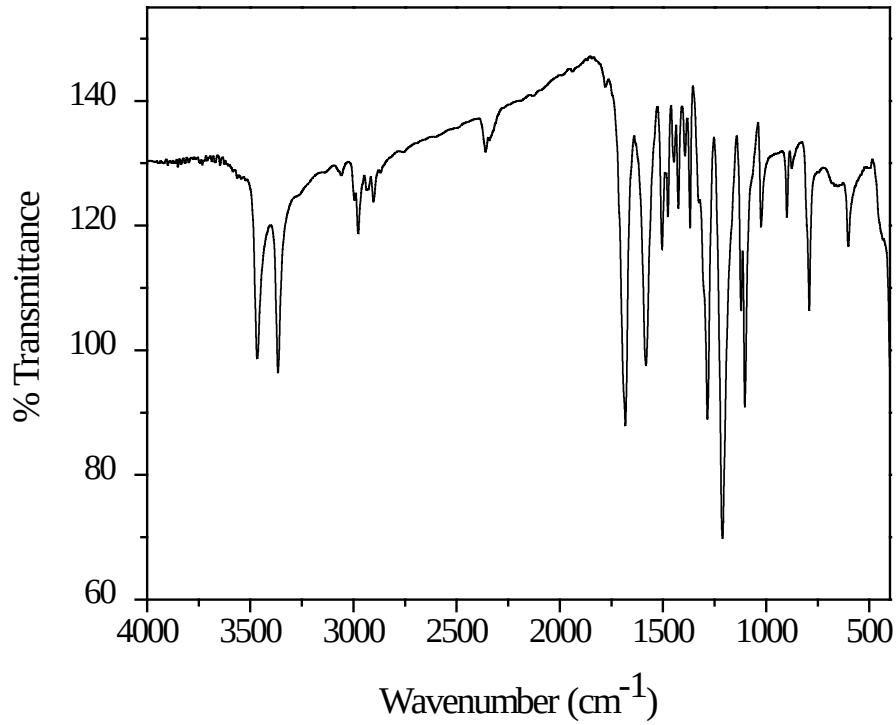

Figure SI6. FTIR of the dye **3** in KBr.

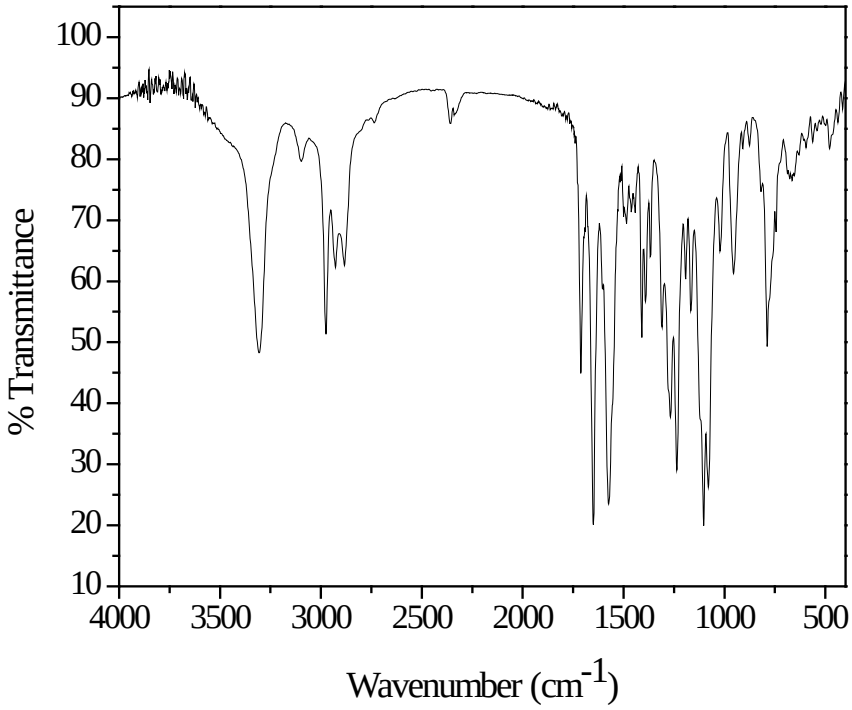

Figure SI7. FTIR of the silsesquioxane **5** in KBr.

2. Theoretical calculations

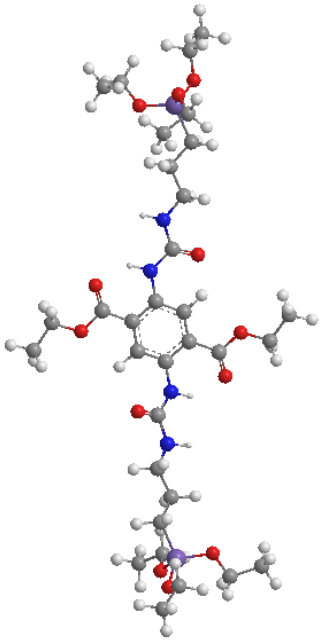

Figure SI8. Theoretical structure of dye **5** optimized at PM3 level.

Table SI1. Bond distances from theoretical calculations.

Atoms	d (Å)	Atoms	D (Å)	Atoms	d (Å)
C(1)-C(2)	1.389	C(19)-C(20)	1.516	C(31)-H(96)	1.111
C(1)-C(6)	1.403	C(19)-H(73)	1.097	C(32)-C(33)	1.506
C(1)-H(108)	1.117	C(19)-H(74)	1.098	C(32)-H(93)	1.110
C(2)-C(3)	1.415	C(19)-H(75)	1.098	C(32)-H(94)	1.115
C(2)-C(14)	1.489	C(20)-H(103)	1.106	C(33)-Si(34)	1.916
C(3)-C(4)	1.399	C(20)-H(104)	1.106	C(33)-H(91)	1.104
C(3)-N(9)	1.432	C(21)-N(22)	1.434	C(33)-H(92)	1.104
C(4)-C(5)	1.396	C(21)-O(35)	1.231	Si(34)-O(39)	1.702
C(4)-H(107)	1.100	N(22)-C(24)	1.486	Si(34)-O(40)	1.701
C(5)-C(6)	1.413	N(22)-H(23)	0.999	Si(34)-O(41)	1.701
C(5)-C(12)	1.487	C(24)-C(25)	1.527	O(37)-C(43)	1.394
C(6)-N(7)	1.425	C(24)-H(101)	1.111	O(38)-C(45)	1.397
N(7)-C(21)	1.422	C(24)-H(102)	1.109	O(39)-C(46)	1.397
N(7)-H(8)	1.014	C(25)-C(26)	1.506	O(40)-C(48)	1.398
N(9)-C(28)	1.427	C(25)-H(99)	1.115	O(41)-C(47)	1.397
N(9)-H(10)	1.013	C(25)-H(100)	1.110	O(42)-C(44)	1.391
O(11)-C(12)	1.355	C(26)-Si(27)	1.916	C(43)-C(52)	1.523
O(11)-C(20)	1.432	C(26)-H(97)	1.104	C(43)-H(89)	1.107
C(12)-O(15)	1.227	C(26)-H(98)	1.104	C(43)-H(90)	1.113
O(13)-C(14)	1.354	Si(27)-O(37)	1.699	C(44)-C(53)	1.523
O(13)-C(18)	1.432	Si(27)-O(38)	1.698	C(44)-H(87)	1.106
C(14)-O(16)	1.226	Si(27)-O(42)	1.702	C(44)-H(88)	1.109
C(17)-C(18)	1.516	C(28)-N(29)	1.437	C(45)-C(54)	1.522
C(17)-H(76)	1.097	C(28)-O(36)	1.227	C(45)-H(85)	1.107
C(17)-H(77)	1.098	N(29)-C(31)	1.485	C(45)-H(86)	1.114
C(17)-H(78)	1.098	N(29)-H(30)	0.999	C(46)-C(51)	1.522
C(18)-H(105)	1.106	C(31)-C(32)	1.527	C(46)-H(83)	1.110
C(18)-H(106)	1.106	C(31)-H(95)	1.109	C(46)-H(84)	1.109
C(47)-C(50)	1.522				

C(47)-H(81)	1.109
C(47)-H(82)	1.115
C(48)-C(49)	1.522
C(48)-H(79)	1.109
C(48)-H(80)	1.109
C(49)-H(70)	1.097
C(49)-H(71)	1.098
C(49)-H(72)	1.098
C(50)-H(67)	1.097
C(50)-H(68)	1.098
C(50)-H(69)	1.098
C(51)-H(64)	1.097
C(51)-H(65)	1.098
C(51)-H(66)	1.098
C(52)-H(61)	1.097
C(52)-H(62)	1.099
C(52)-H(63)	1.098
C(53)-H(58)	1.097
C(53)-H(59)	1.104
C(53)-H(60)	1.099
C(54)-H(55)	1.097
C(54)-H(56)	1.098
C(54)-H(57)	1.098

3. X-ray diffraction

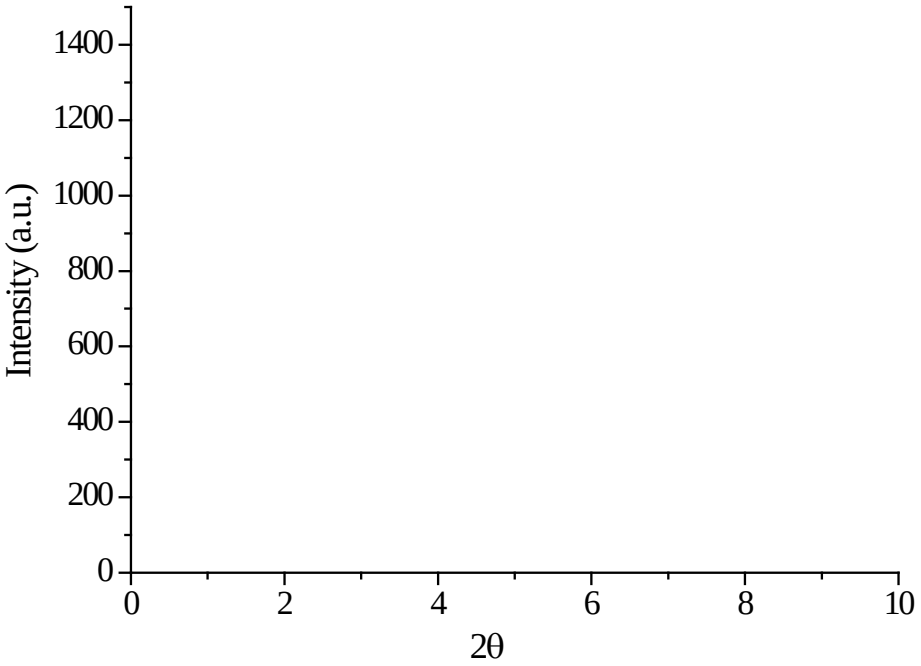

Figure SI9. X-ray diffraction patterns of the **DPM1**.

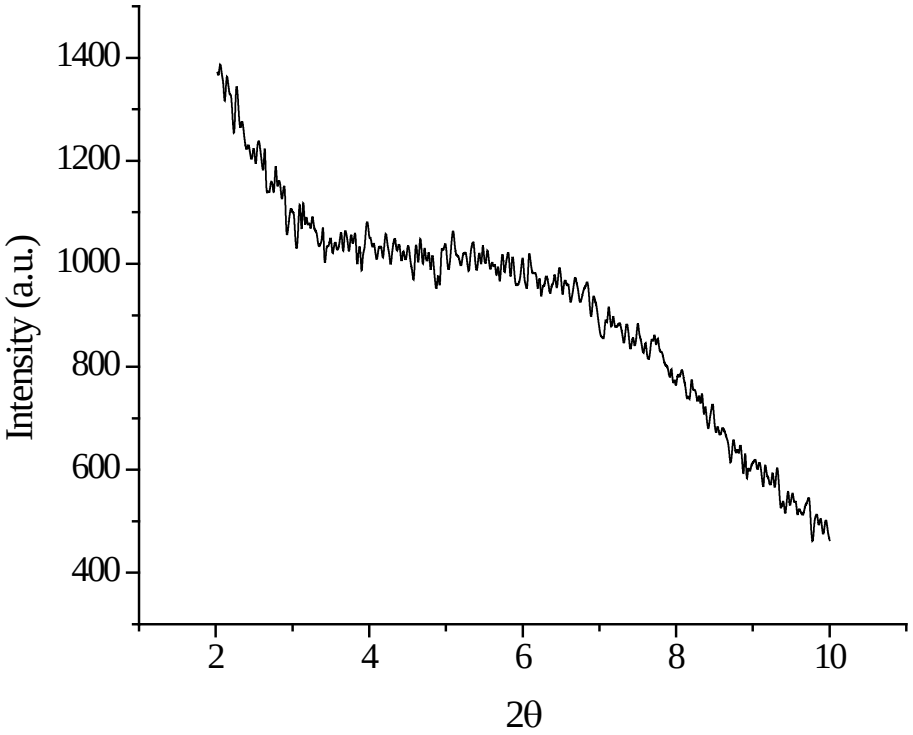

Figure SI10. X-ray diffraction patterns of the **DPM2**.

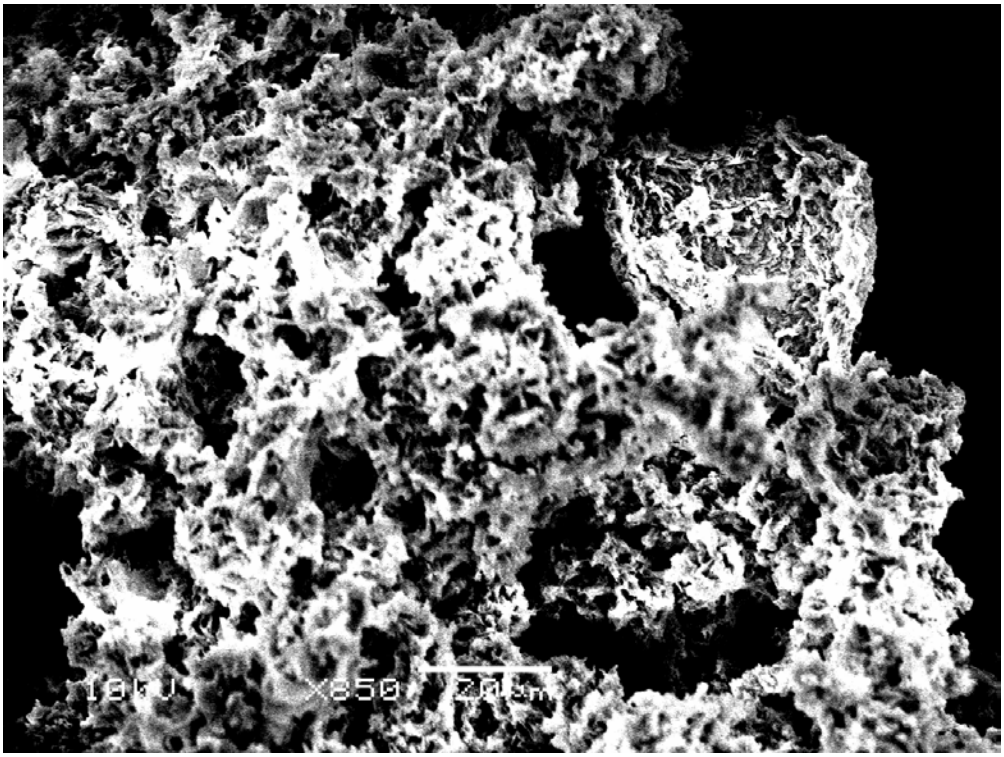

Figure SI11. SEM picture of the **DPM1**.

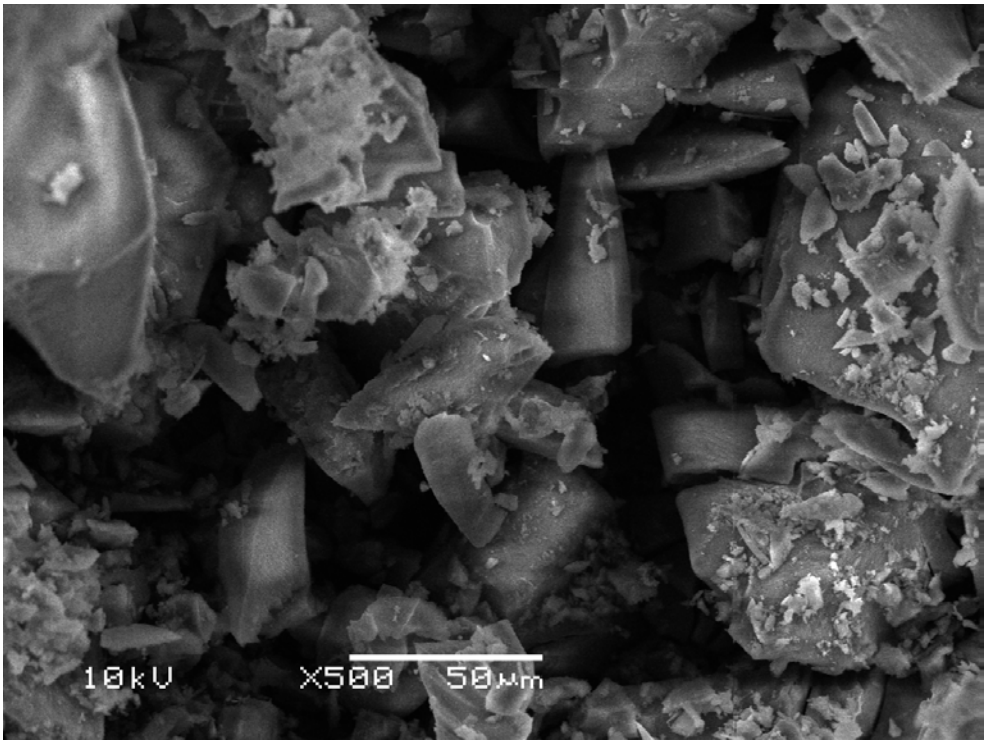

Figure SI12. SEM picture of the **DPM2**.

4. Excitation Spectra

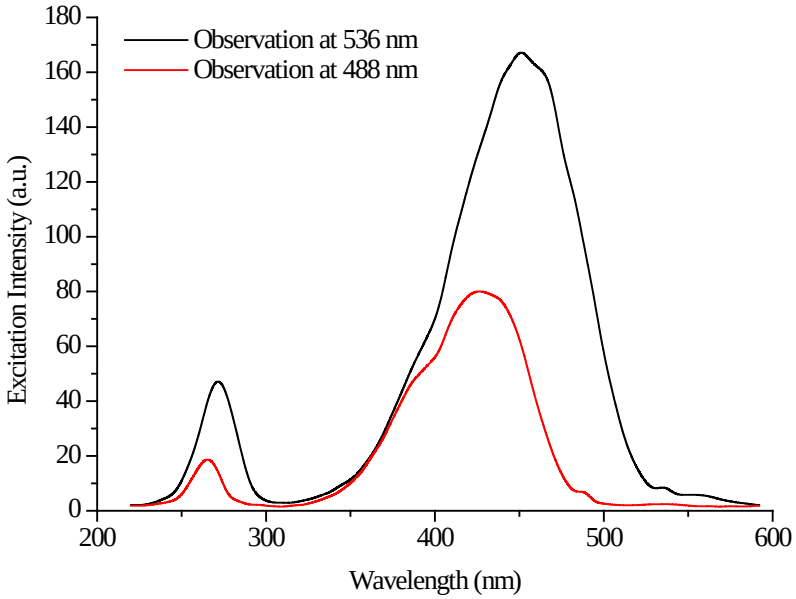

Figure SI13. Excitation spectra of dye **3** in 1,4-dioxane at two different observation wavelengths 536 nm and 488 nm.

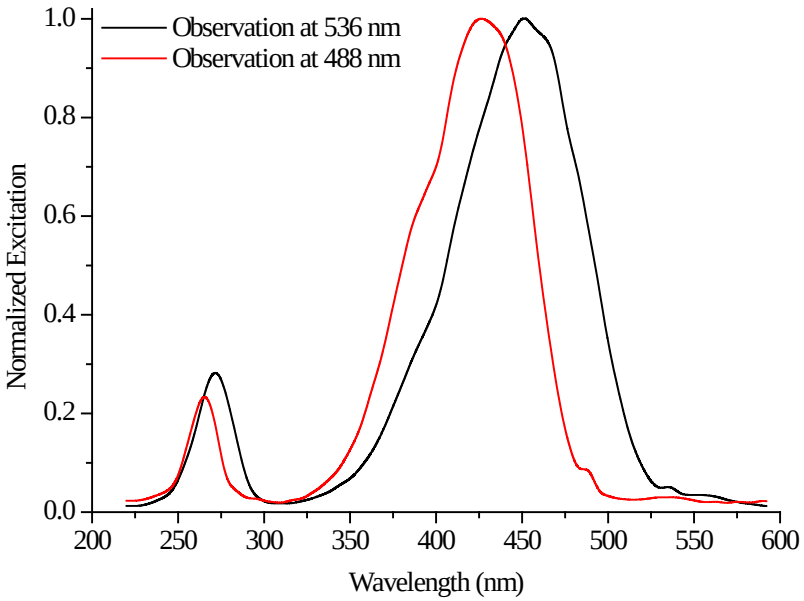

Figure SI14. Normalized excitation spectra of dye **3** in 1,4-dioxane at two different observation wavelengths 536 nm and 488 nm.

5. Time Resolved Fluorescence Experiments

Table SI2. Experimental data from the time resolved fluorescence spectroscopy.

Dye	Abs.	Slit (nm)	Led (nm)	cut-on filter (nm)	Start (ns)	End (ns)	Channels	Integration time (s)	Average
3	0.502	0.30	405	400	45	500	250	1	2
5	0.088	0.40	380	380	55	400	172	1	3

Table SI3. Relevant data from the time resolved fluorescence spectroscopy.

Dye	a_1	τ_1 (ns)	a_2	τ_2 (ns)	χ^2
3	0.4596	15.06 ± 6.217e-002	0.9332	0.04683 ± 1.685e+000	1.117
5	0.4748	9.295 ± 3.637e-001	-	-	1.033

6. Thermogravimetric Analysis

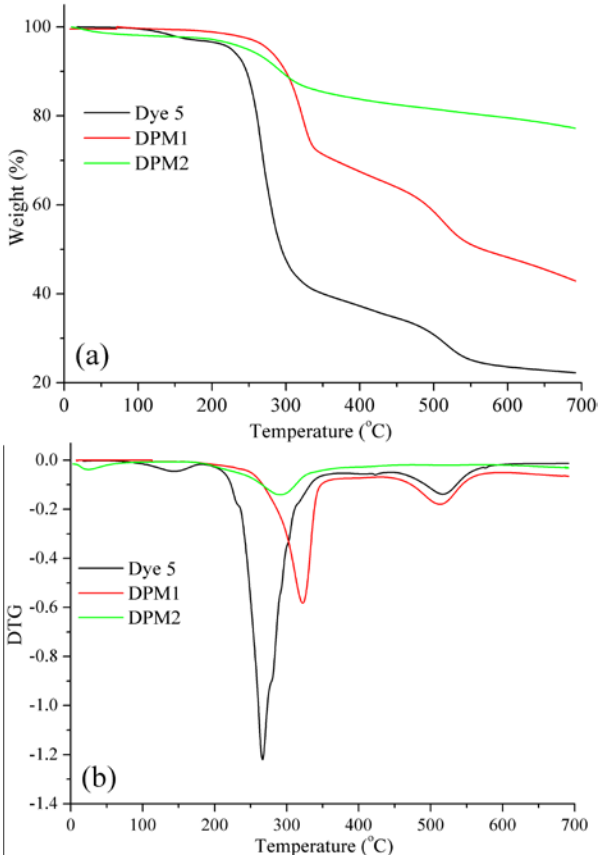

Figure SI14. (a) TGA and (b) DTG curves of dye **5** and the obtained materials **DPM1** and **DPM2**.