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New Journal of Chemistry

Electronic Supplementary Information for

Magnetic nanoparticles with chelating shells prepared by RAFT/MADIX polymerization

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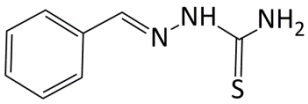
Benzaldehyde thiosemicarbazone (BTSC) analyses



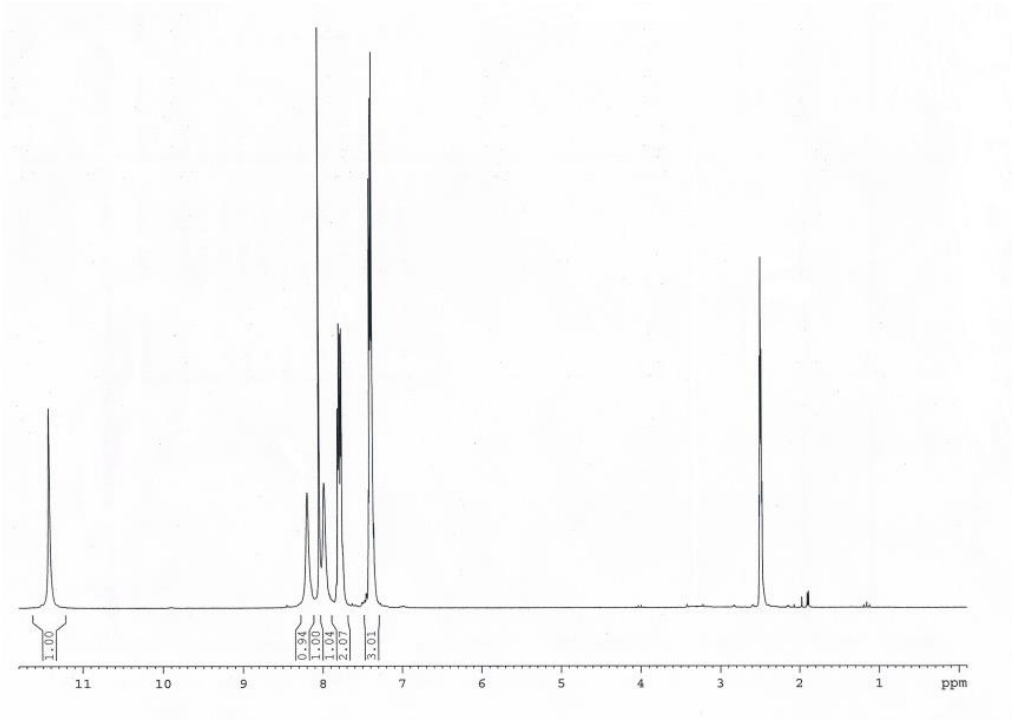


Fig. S1 ^{1}H NMR spectrum of benzaldehyde thiosemicarbazone (BTSC).

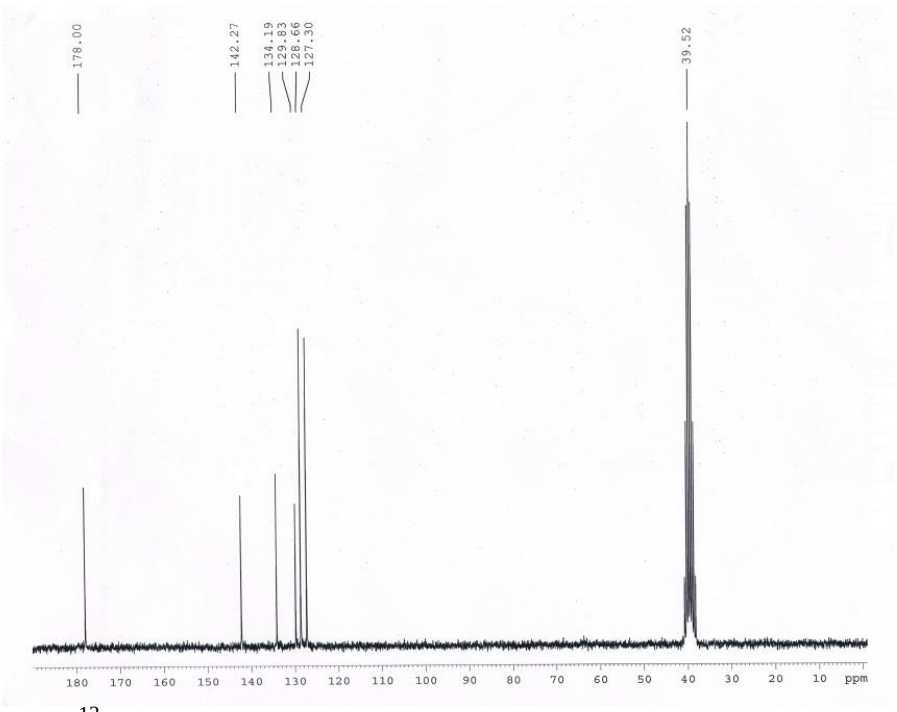
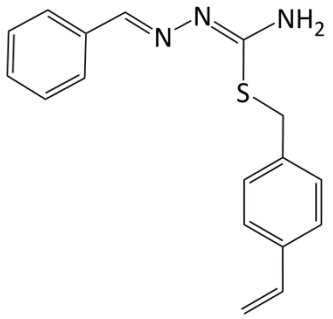


Fig. S2 ^{13}C NMR spectrum of benzaldehyde thiosemicarbazone (BTSC).

Bifunctional monomer (BM) analyses



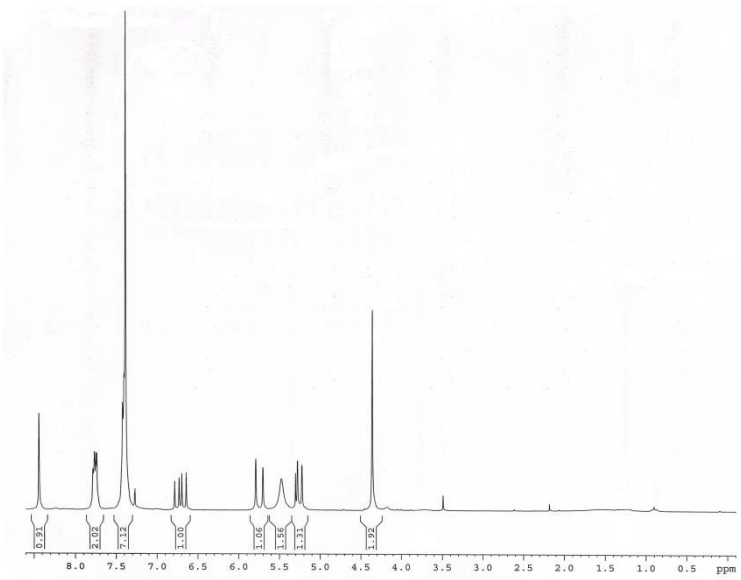


Fig. S3 ^{1}H NMR spectrum of product bifunctional monomer (BM).

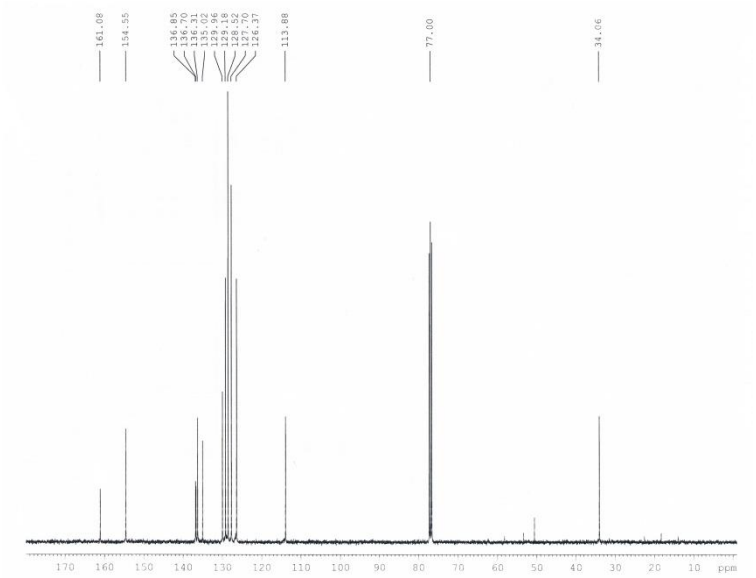


Fig. S4 ^{13}C NMR spectrum of bifunctional monomer (BM).

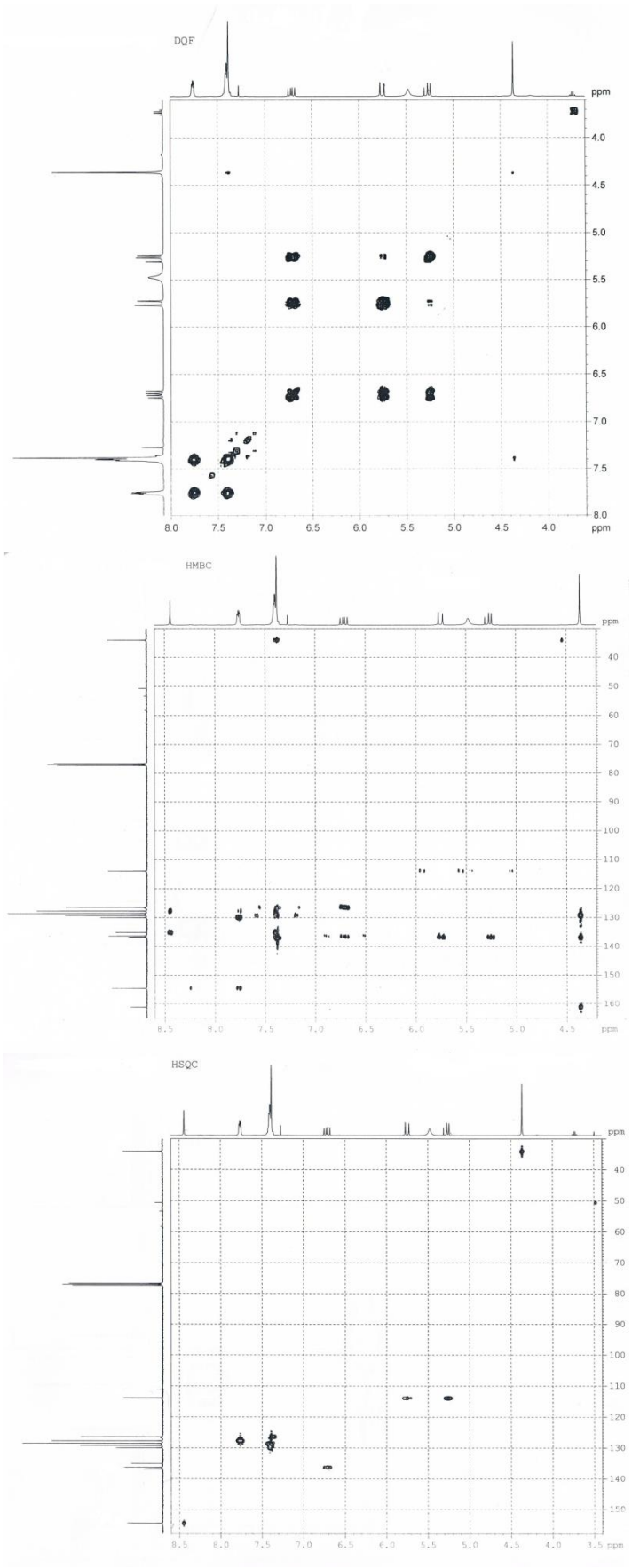


Fig. S5 2D NMR spectra of bifunctional monomer (BM).

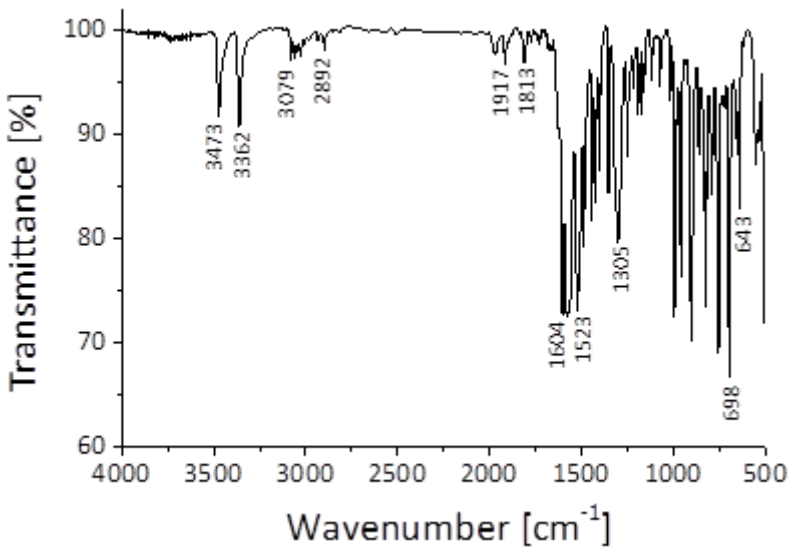


Fig. S6 FT IR spectrum of bifunctional monomer (BM).

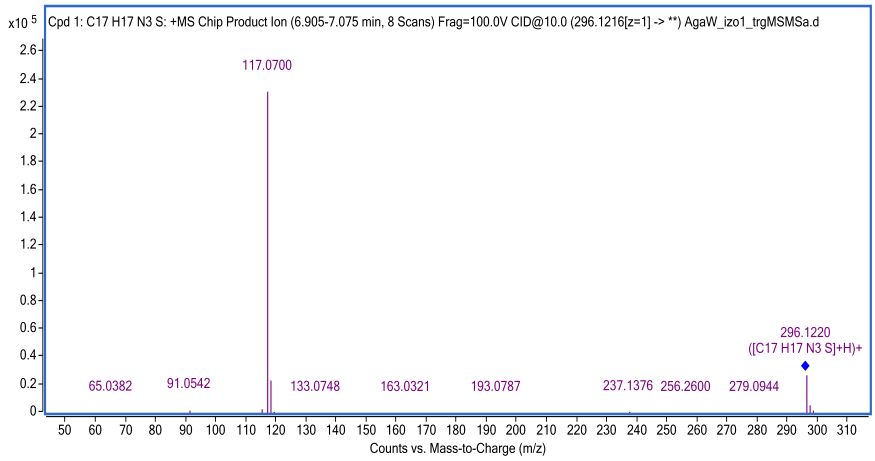


Fig. S7 LC-ESI-CID-Q/TOF spectrum of bifunctional monomer (BM); collision energy: 10eV.

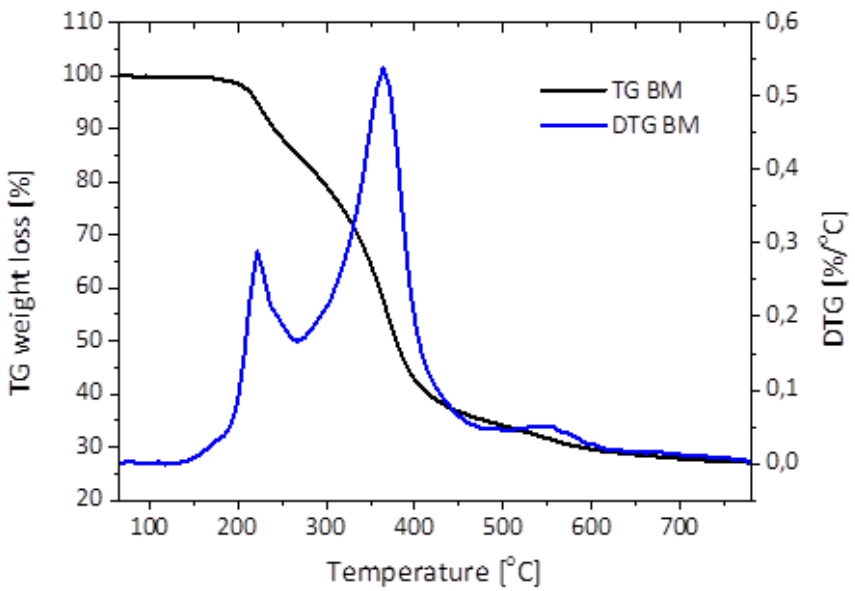
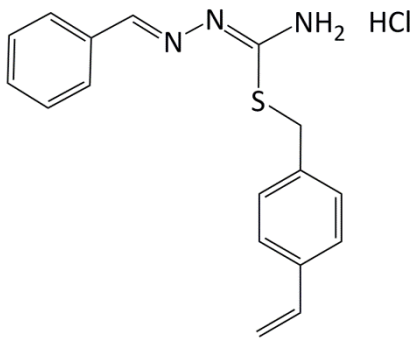


Fig. S8 TG and DTG curves of BM.

Bifunctional monomer salt (BMS) analyses



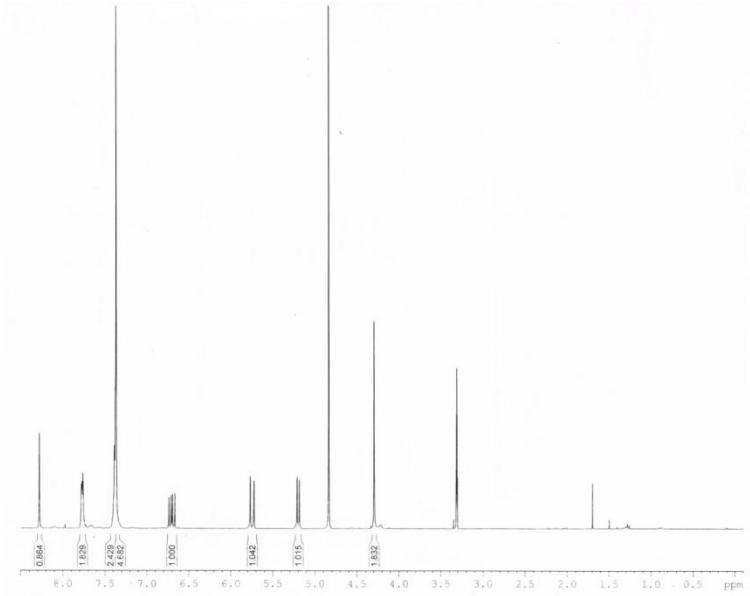


Fig. S9 ^{1}H NMR spectrum of bifunctional monomer salt (BMS).

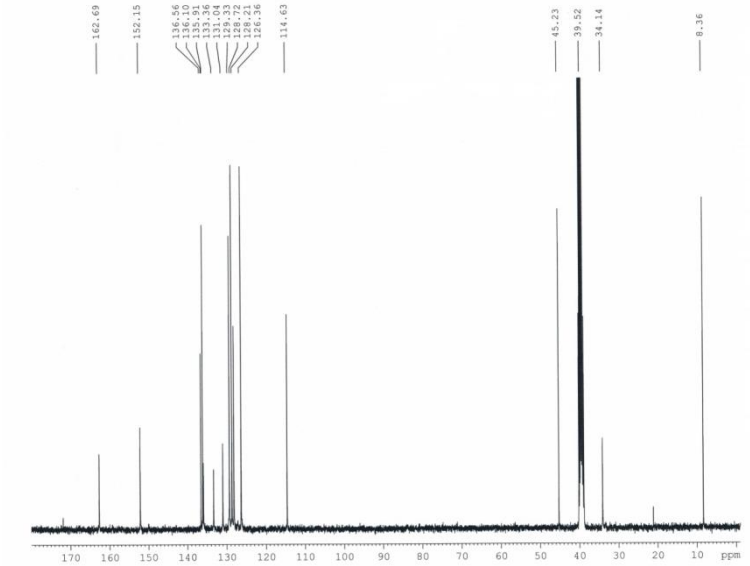


Fig. S10 ^{13}C NMR spectrum of bifunctional monomer salt (BMS).

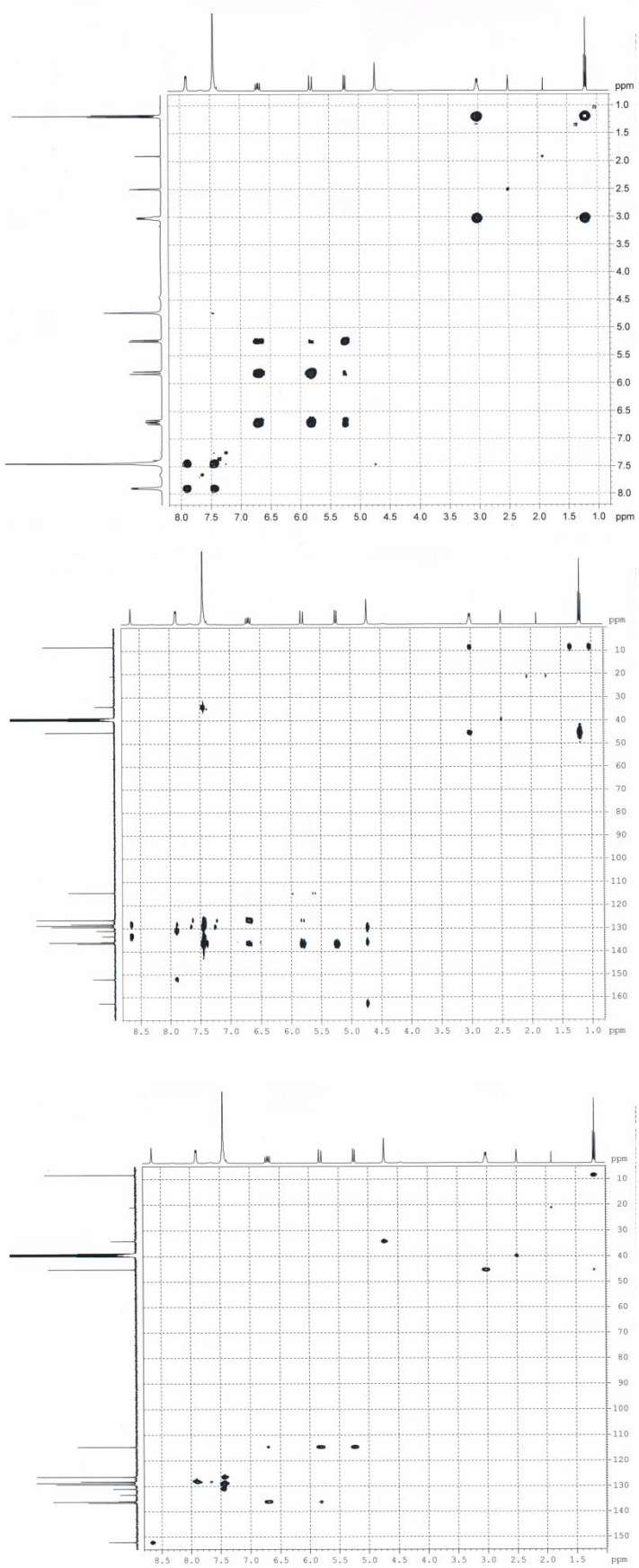


Fig. S11 2D NMR spectra of bifunctional monomer salt (BMS).

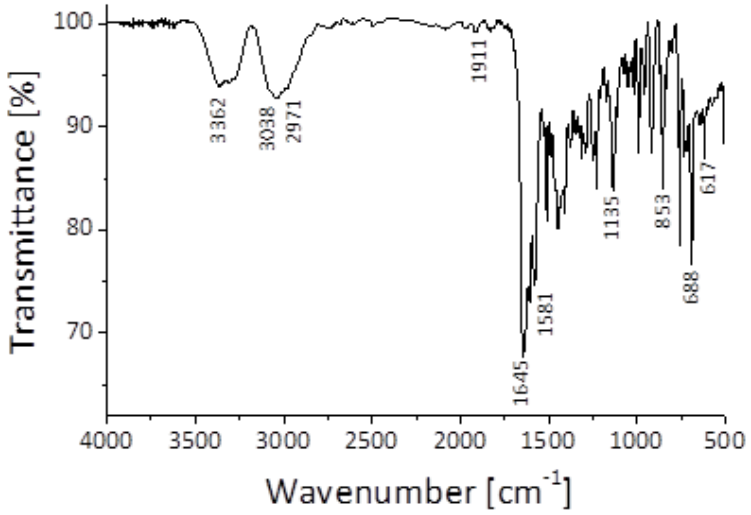


Fig. S12 FT IR spectrum of bifunctional monomer salt (BMS).

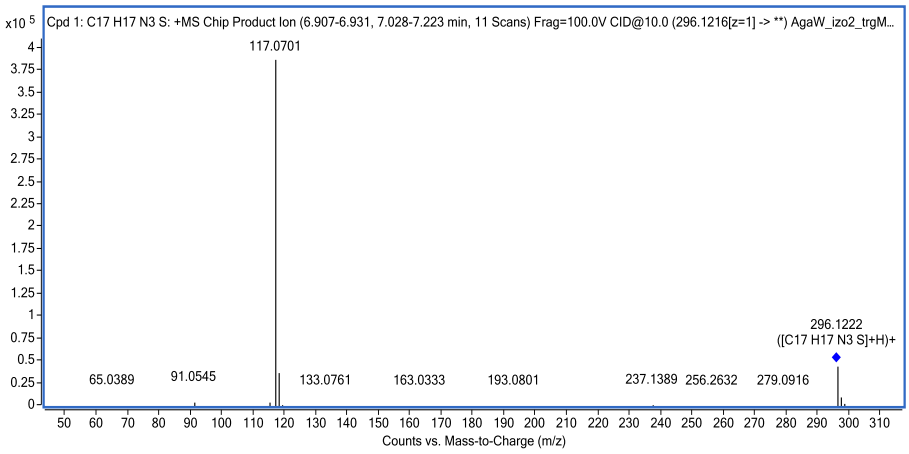


Fig. S13 LC-ESI-CID-Q/TOF spectra of bifunctional monomer salt (BMS); collision energy: 10eV.

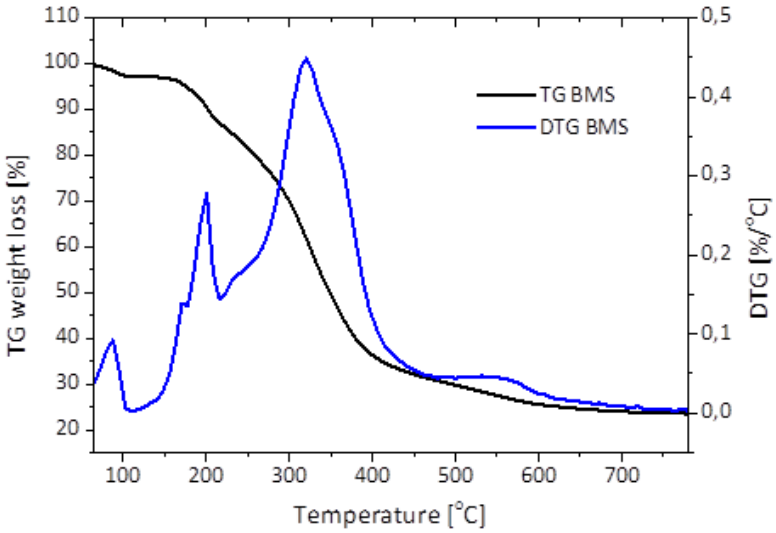


Fig. S14 TG and DTG curves of BMS.

Table S1 Crystal data and structure refinement for BM and BMS.

	BM	BMS
Empirical formula	$C_{17}H_{17}N_3S$	$C_{17}H_{18}N_3S^{1+}$, $C_1H_4O_1$, Cl^{1-}
Formula weight, g mol^{-1}	295.41	363.90
Crystal size/mm^3	0.484 × 0.422 × 0.040	0.298 × 0.213 × 0.093
Crystal system	triclinic	triclinic
Space group	$P\bar{1}$	$P\bar{1}$
a/Å	8.665(7)	9.417(6)
b/Å	9.386(5)	10.225(6)
c/Å	10.489(7)	11.86(4)
α/°	84.169(2)	67.799(2)
β/°	87.261(12)	68.787(2)
γ/°	64.997(2)	66.310(2)
Volume/$Å^3$	769.26(4)	938.49(4)
Z	2	2
ρ_{calc}g/cm^3	1.2753	1.288
μ/mm^{-1}	0.207	0.324
Temperature/K	100	100
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
Completness (%)	99.7	99.9
2Θ range/°	5.92 to 72.62	5.54 to 72.64
Reflections collected	37171	45409
Independent reflections	7441 [R_{int} = 0.0412, R_{sigma} = 0.0269]	9081 [R_{int} = 0.0463, R_{sigma} = 0.0338]
parameters /restraints	205/0	230/0
Goodness-of-fit on F^2	1.098	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0404, wR_2 = 0.1062	R_1 = 0.0446, wR_2 = 0.1116
Final R indexes [all data]	R_1 = 0.0519, wR_2 = 0.1179	R_1 = 0.0656, wR_2 = 0.1258
Largest diff. peak/hole / e $Å^{-3}$	0.66/-0.30	0.72/-0.34

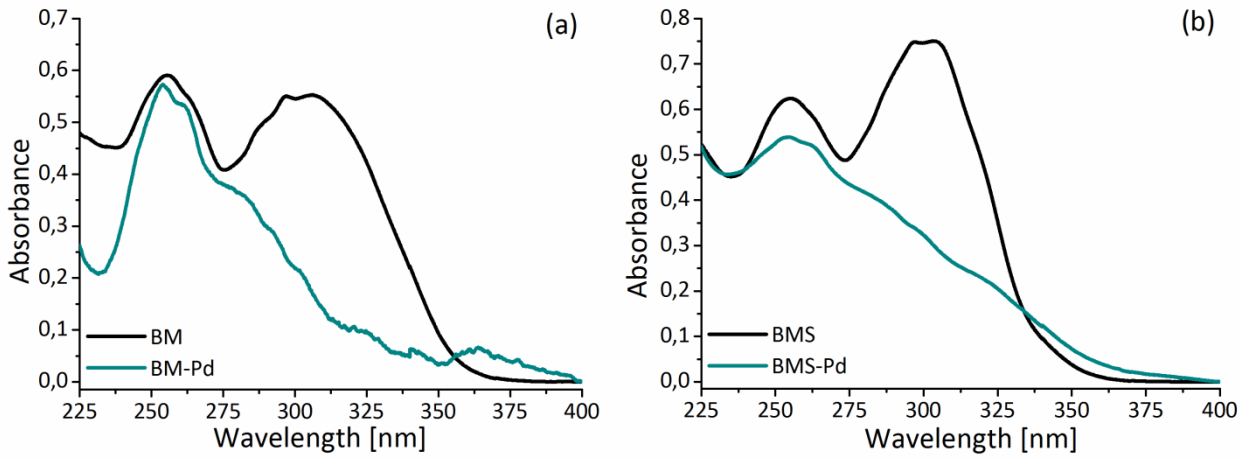


Fig. S15 UV spectra of (a) BM and BM-Pd, (b) BMS and BMS-Pd (normalized to 1).

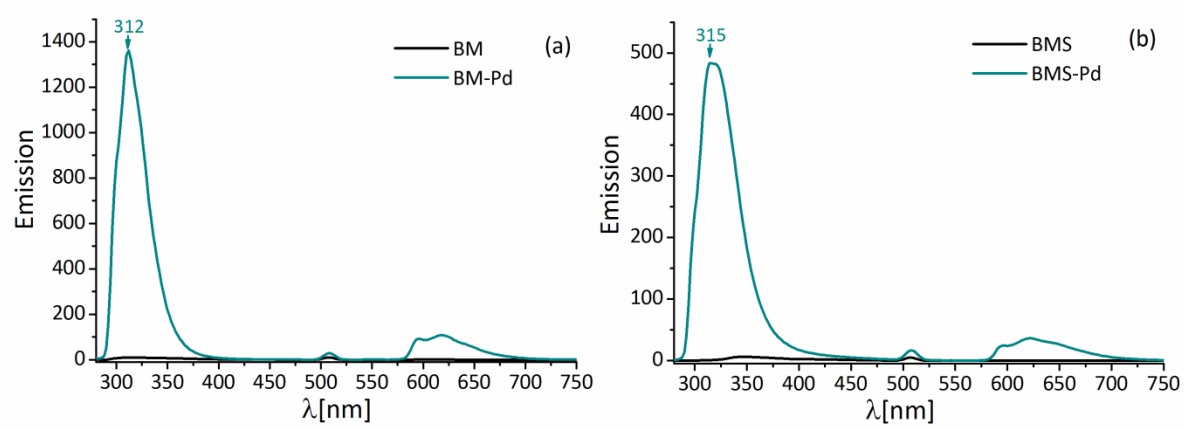


Fig. S16 Fluorescence spectra of (a) BM-M and (b) BMS-M.