Achievement of enhanced solubility and improved optics in the molecular complexes based on sulfonate-pyridinium supramolecular synthon

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KEYWORDS: Co-crystal, molecular salt, solubility, optical properties

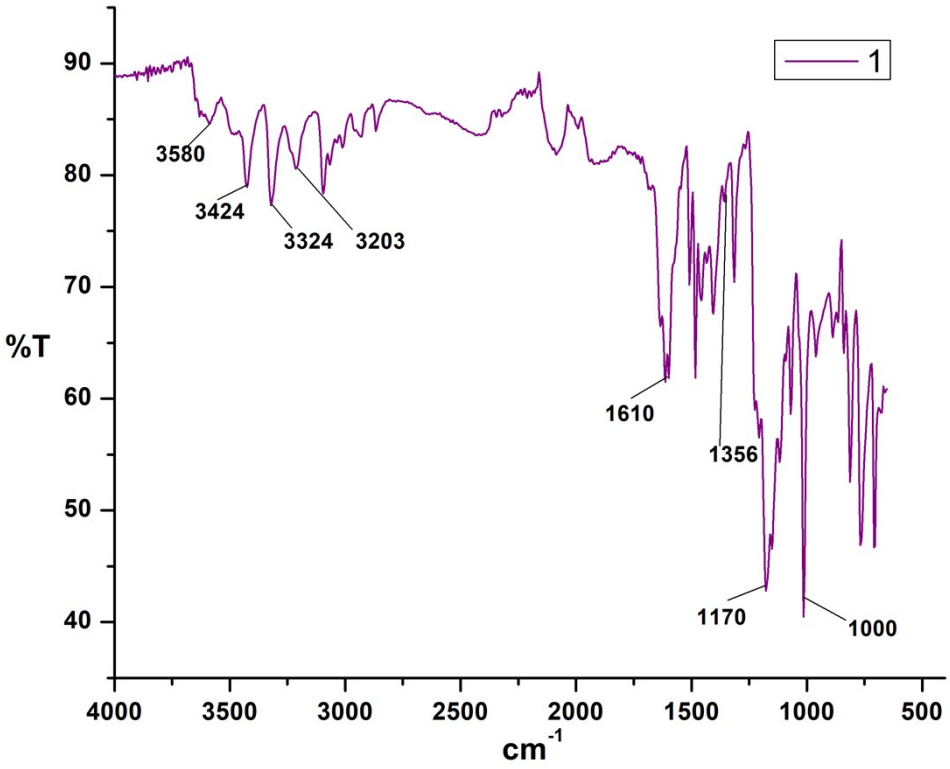

Fig. ESI-1 FT-IR Spectrum of **1.**

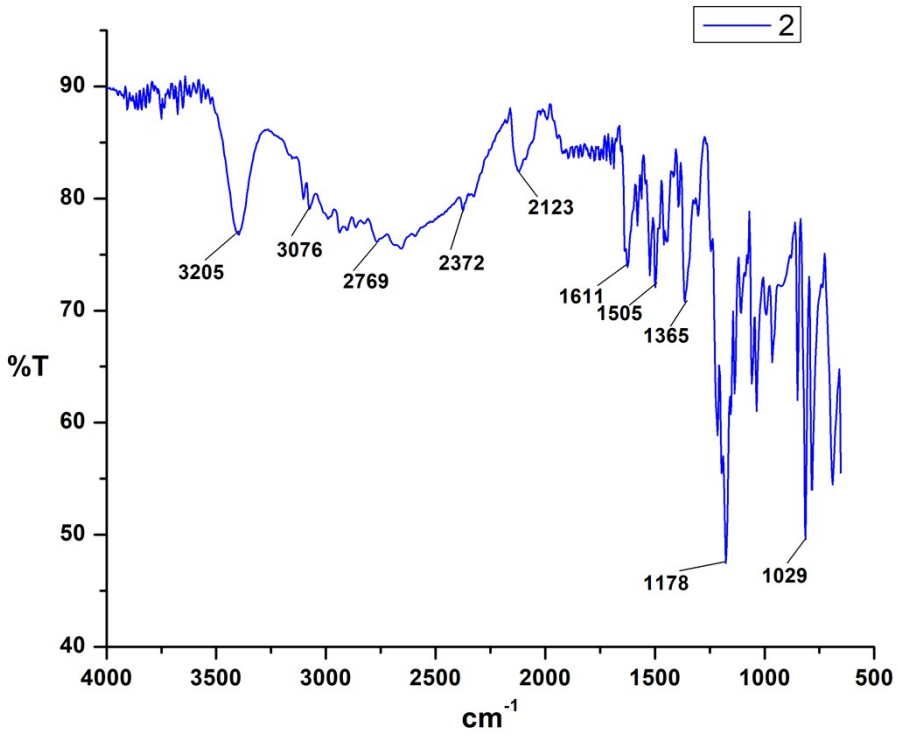

Fig. ESI-2 FT-IR Spectrum of **2.**

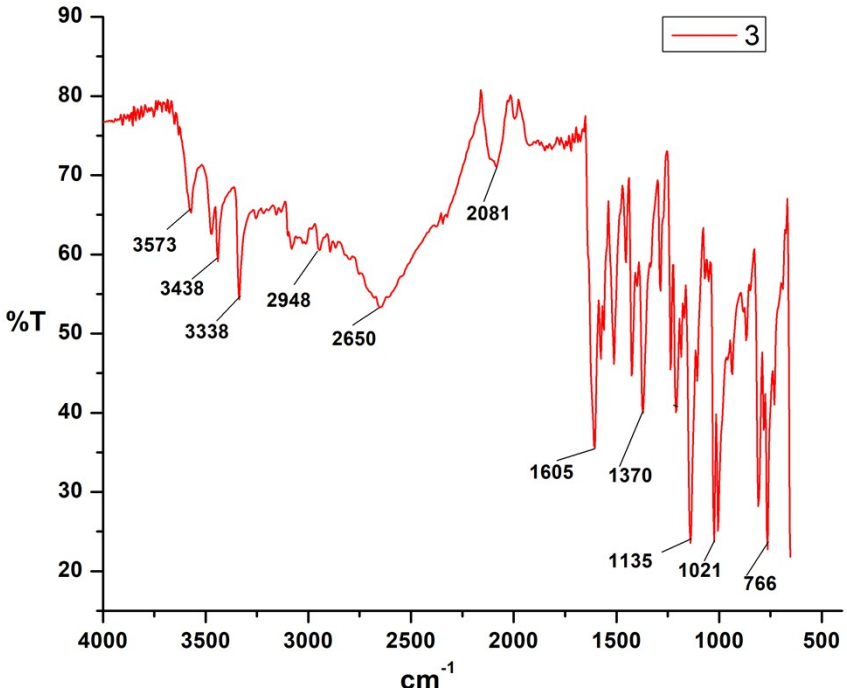

Fig. ESI-3 FT-IR Spectrum of **3.**

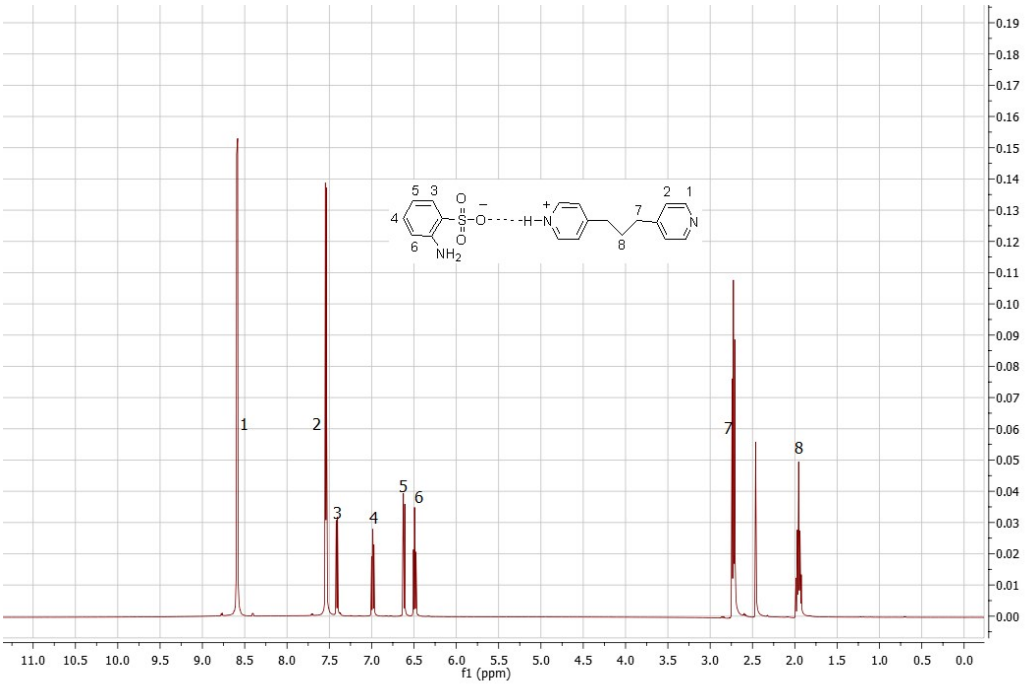

Fig. ESI-4 1H NMR Spectrum of **1** reported in DMSO-*d6* at 400 MHz.

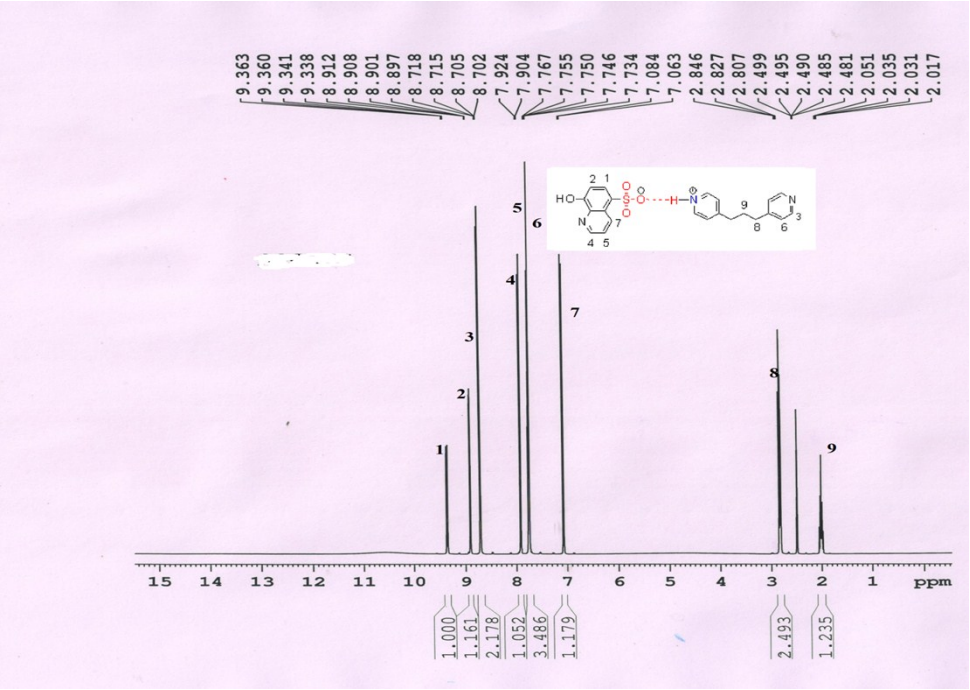

Fig. ESI-5 1H NMR Spectrum of **2** reported in DMSO-*d*6 at 400 MHz.

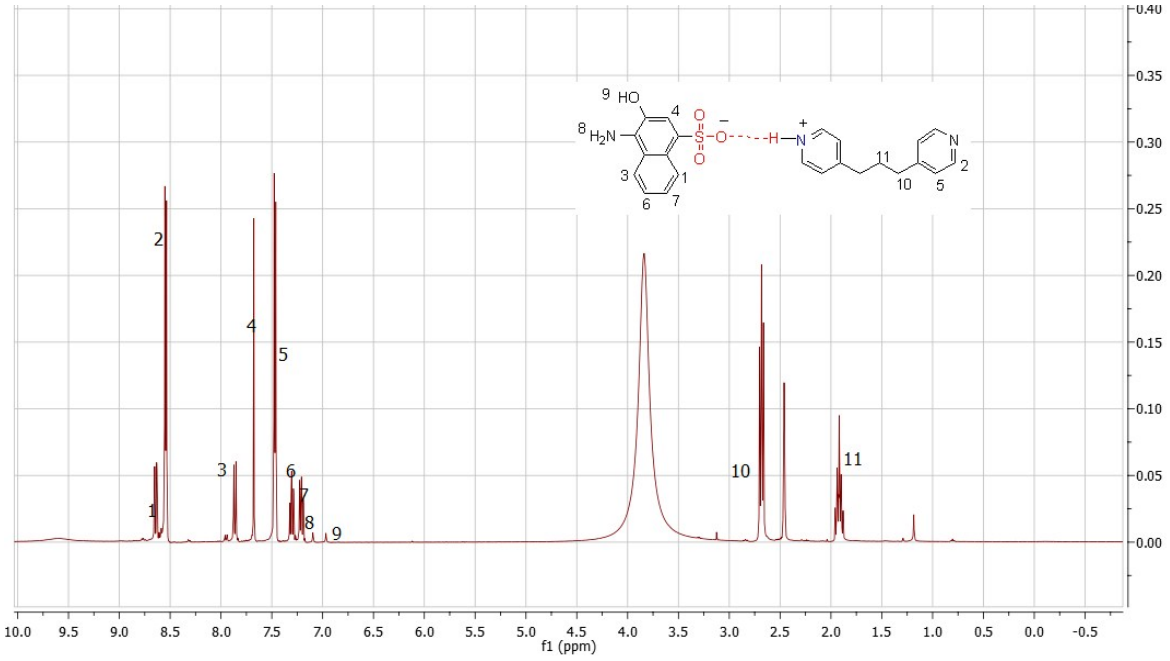

Fig. ESI-6 1H NMR Spectrum of **3** reported in DMSO-*d*6 at 400 MHz.

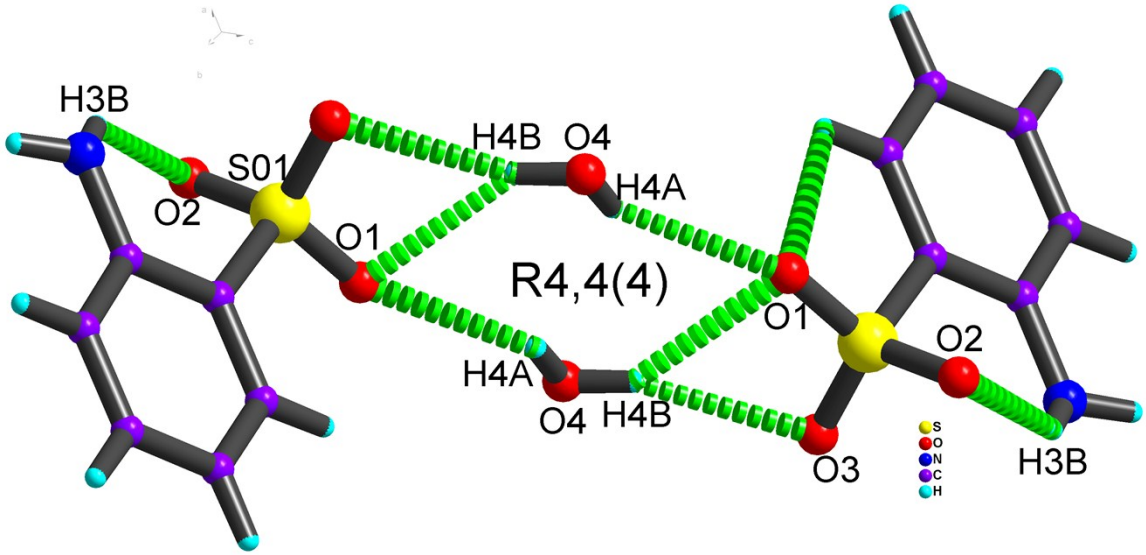

Fig ESI-7 Centro-symmetric hydrated amino-aryl sulfonate dimer in **1**.

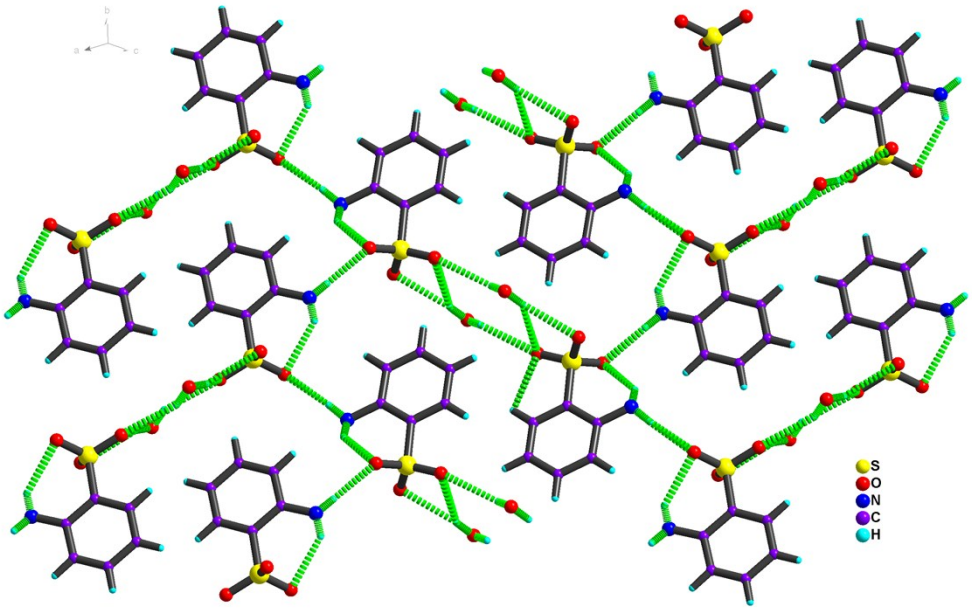

Fig. ESI-8 Anionic hydrated layers of amino-aryl sulfonate dimer in **1**.

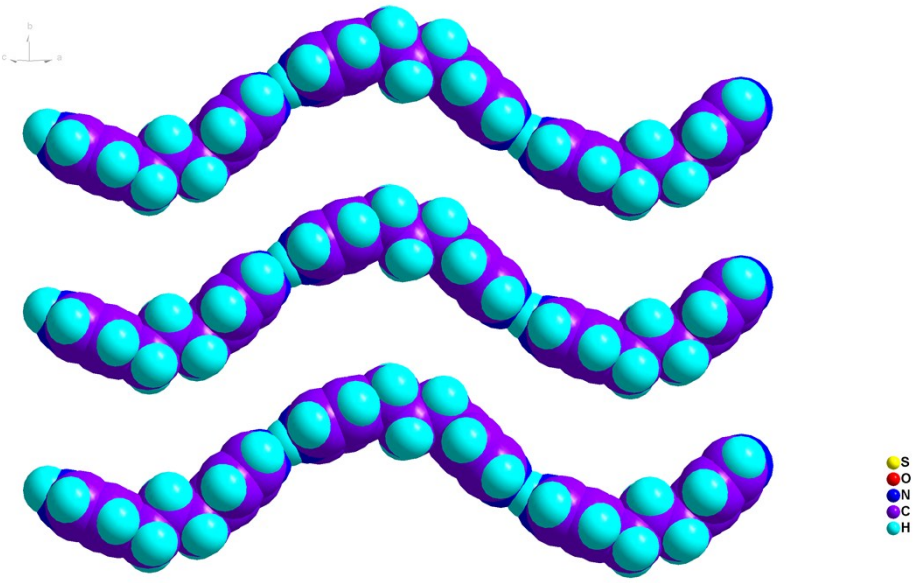

Fig. ESI-9 Isolated bis-pyridinium chains in **1.**

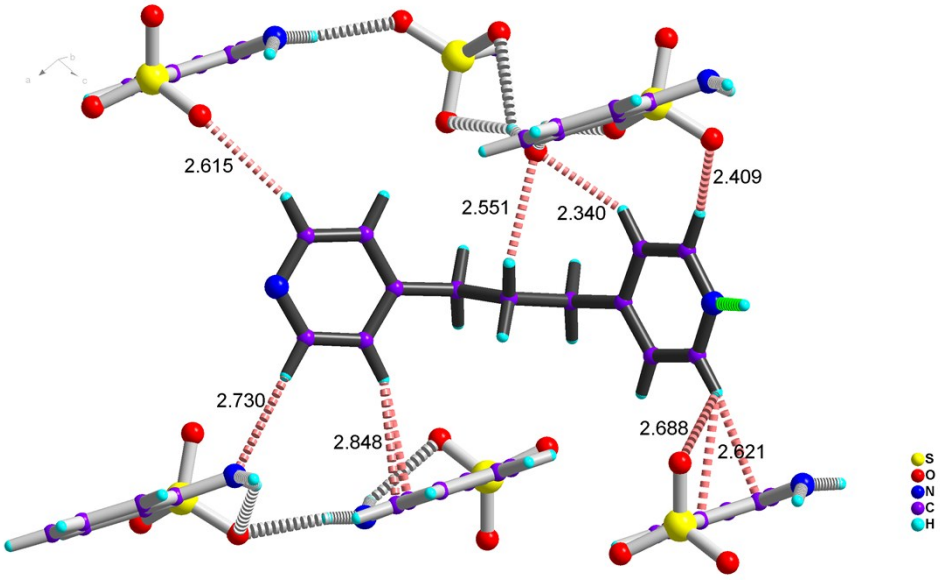

Fig. ESI-10 Interactions between bis-pyridinium chains and anionic layers of amino-aryl sulfonate layers in **1.**

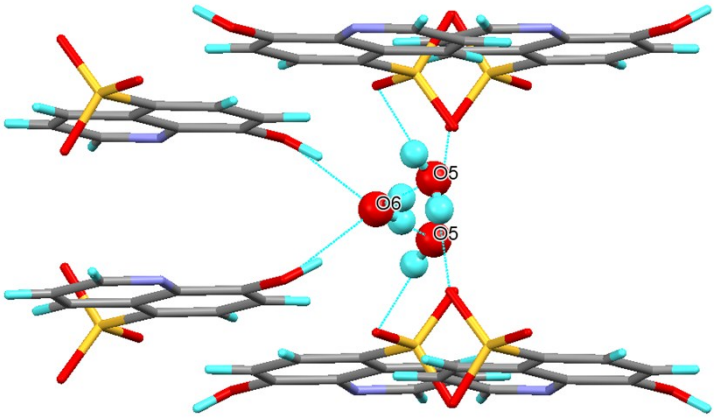

Fig. ESI-11 Hexa-sulfonate:tri-aqua clusters in **2**.

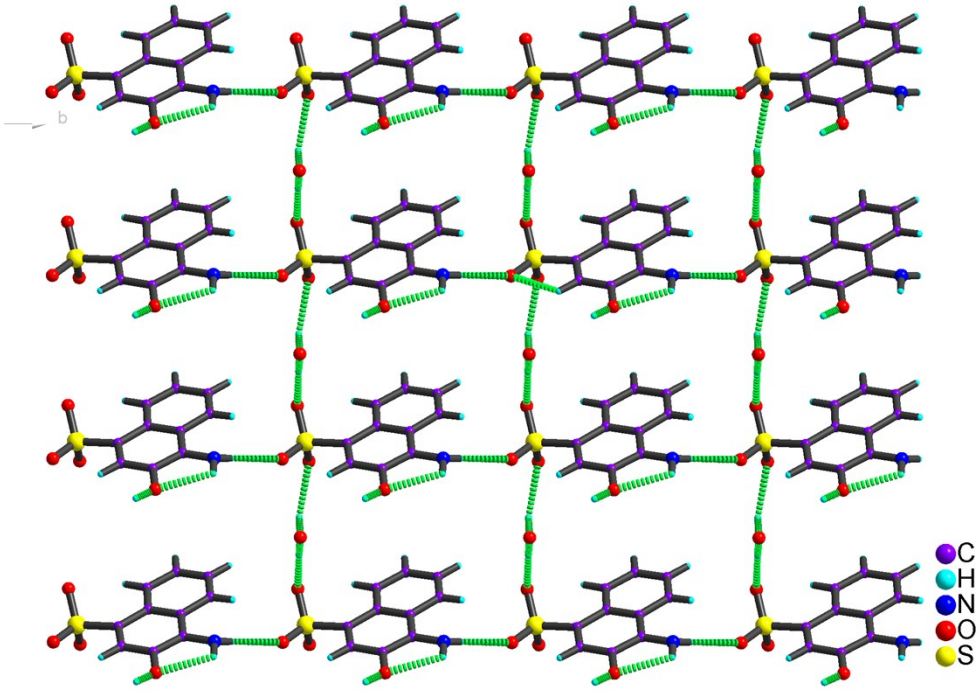

Fig. ESI-12 2-D hydrated anionic nets of organo-sulfonates in **3**.

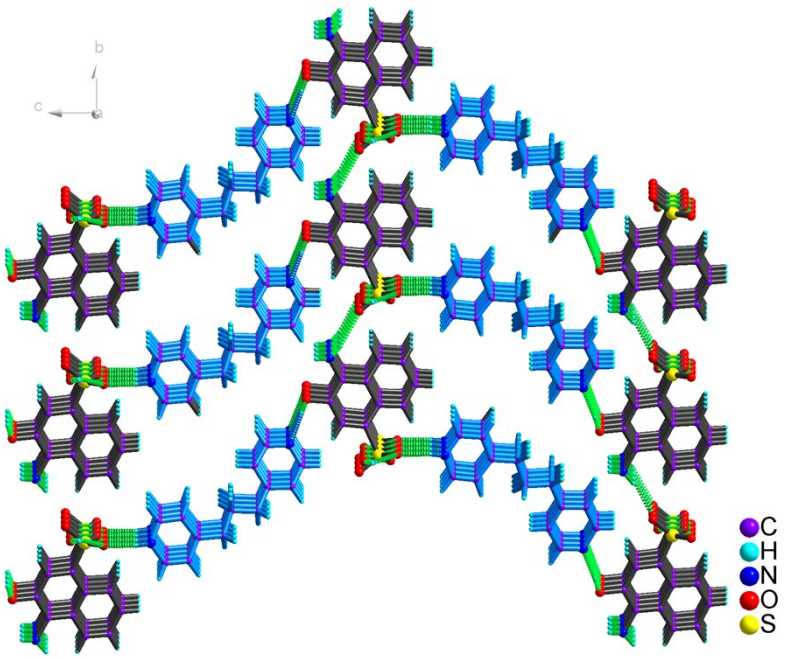

Fig. ESI-13 3-D reticular nets formed in 3 by briding of anionic layers of hydrated organo-sulfonate leayers by 4,4'-BPP in **3**.

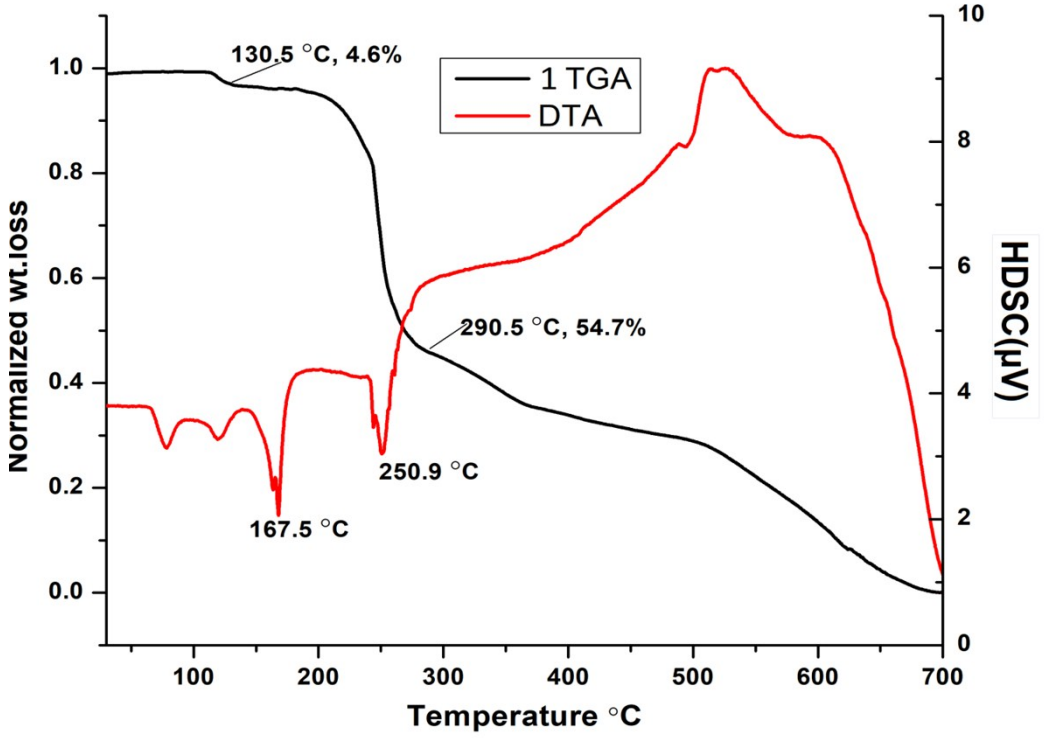

Fig. ESI-14 TGA-DSC curves of **1**.

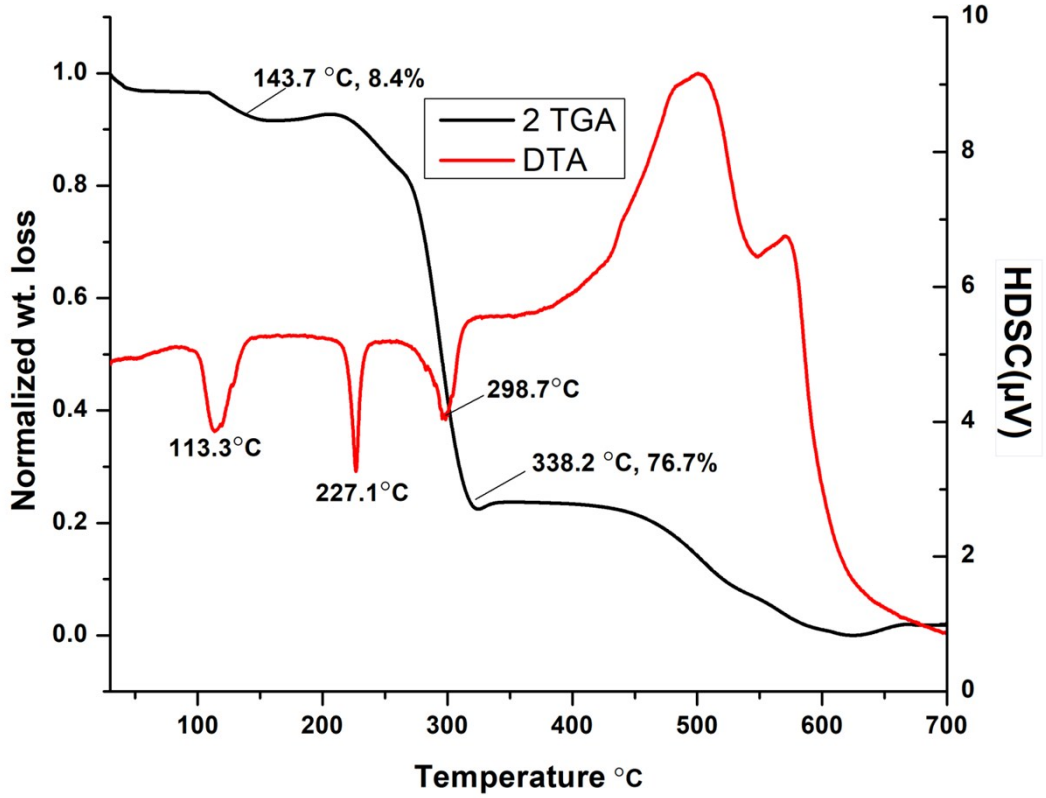

Fig. ESI-15 TGA-DSC curves of **2**.

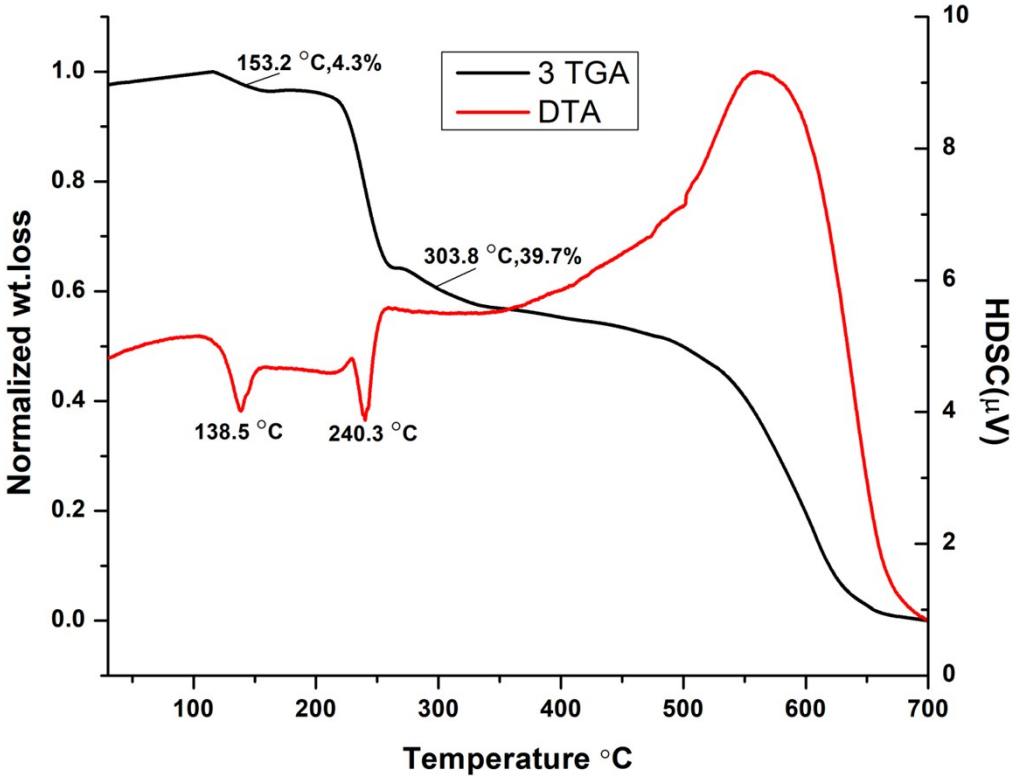

Fig. ESI-16 TGA-DSC curves of **3**.

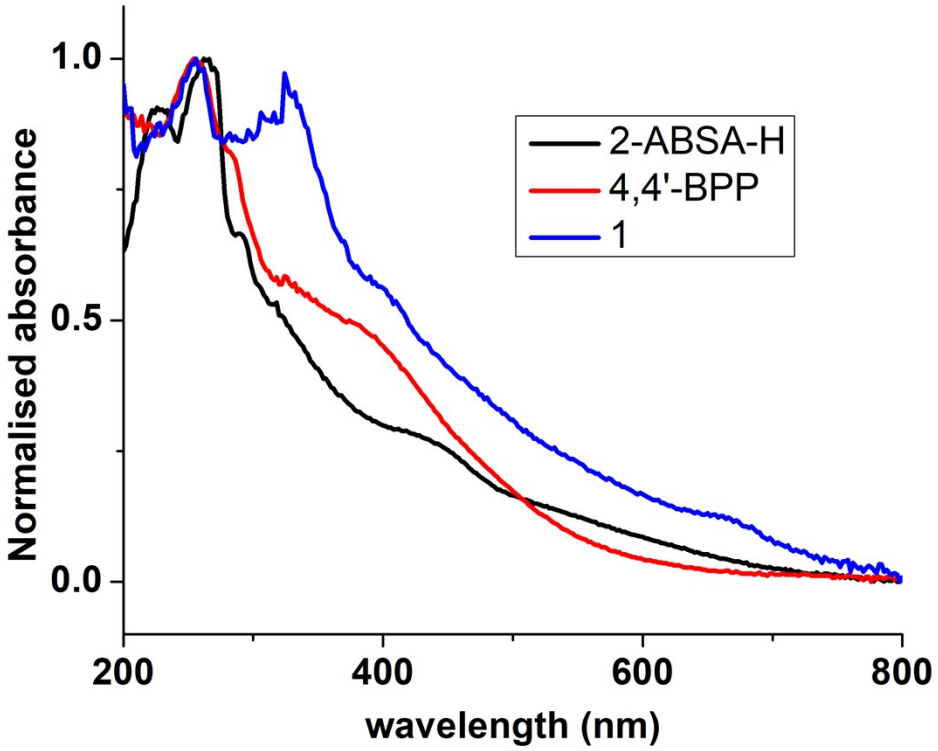

Fig. ESI-17 DR-UV-Vis spectra of starting materials and Compound **1.**

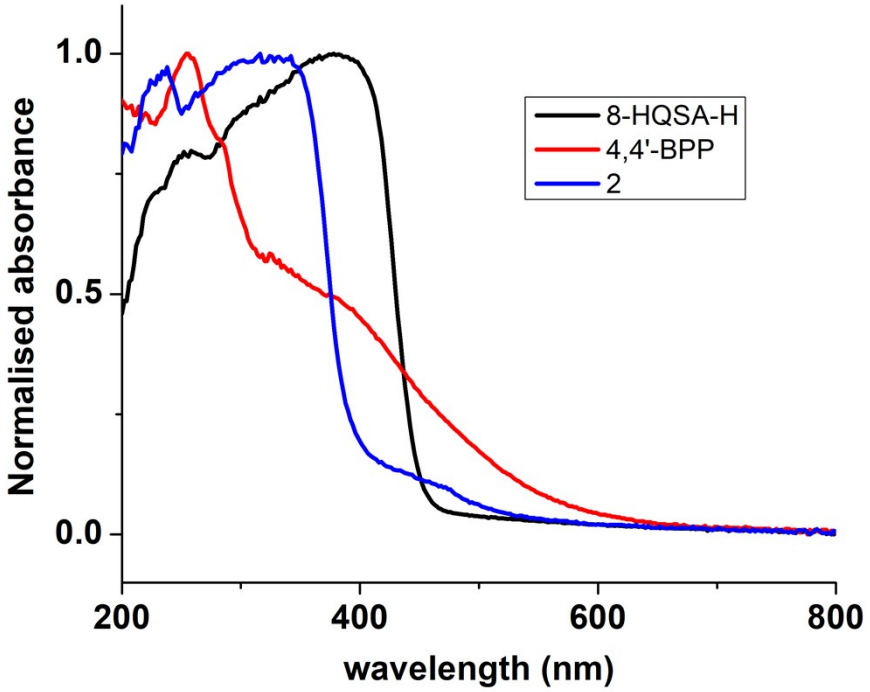

Fig. ESI-18 DR-UV-Vis spectra of starting materials and Compound **2.**

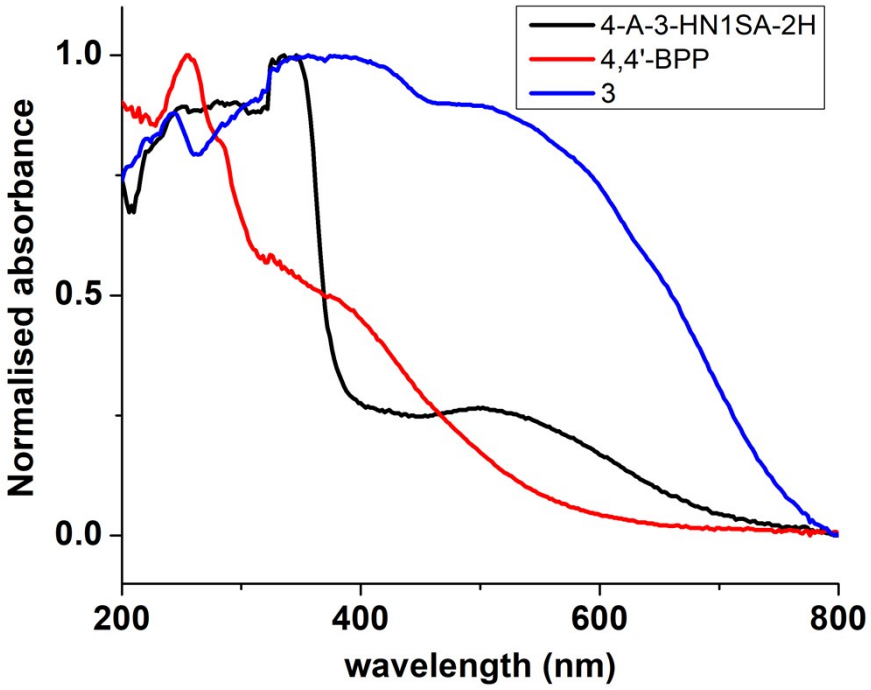

Fig. ESI-19 DR-UV-Vis spectra of starting materials and Compound **3.**

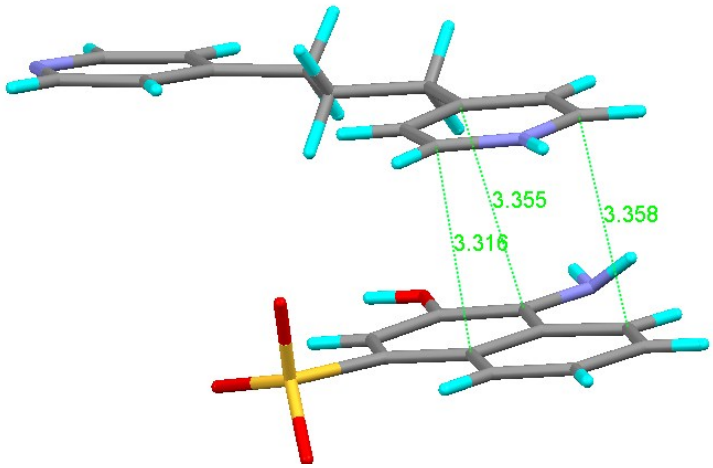

Fig. ESI-20 Strong π-π interactions between crystal formers of **3**.

Table ESI-1. Comparative MPs of formers with molecular salts**.**

Acid former	MP. °C	Base former	MP. °C	Molecular salt	MP. °C
$C_6H_7NO_3S$	>300	$C_{13}H_{14}N_2$	60	1	150
$C_9H_7NO_3S$	>300	$C_{13}H_{14}N_2$	60	2	205
$C_{10}H_{710}NO_4S$	285	$C_{13}H_{14}N_2$	60	3	140

Table ESI-2. Solubility of compounds **1-3** in different solvents

Compound	$CHCl_3$	Acetone	MeOH	EtOH	CH_3CN	DCM	H_2O	DMSO
1	insoluble	insoluble	soluble	soluble	insoluble	partial	soluble	soluble
2	insoluble	insoluble	soluble	soluble	insoluble	partial	soluble	soluble
3	insoluble	insoluble	insoluble	insoluble	insoluble	insoluble	soluble	soluble