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Electronic Supplementary Information (ESI)

Self- assembled supramolecular structure of N,N,N′,N′-tetramethylethylenediammonium-bis-(4-nitrophenolate):synthesis, single crystal growth and photo physical properties

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1. Experimental procedure

1.1 Solubility determination of TMEDA4NP

25 ml of acetonitrile was taken in a pre-weighed clean beaker and kept in constant temperature bath (25°C, ± 0.01°C) with an immersible magnetic stirrer facility. The powdered TMEDA4NP was added slowly to the solvent and stirred well until the saturation ceases. The beaker was taken out and weighed again. The weight of the solution was assessed by taking the difference between the empty beaker and the beaker containing the saturated solution. The solution was then allowed to evaporate and the amount of the solute was determined. The solubility of the material was estimated using the formula

$$Solubility\ (wt\%) = \frac{Weight\ of\ the\ solute}{Weight\ of\ (solute + solvent)} \times 100$$

The above procedure was repeated for five different temperatures (30, 35, 40, 45 and 50°C) and also for determining the solubility of TMEDA4NP in methanol.

Table S1 Bond lengths [Å] and angles [°] for TMEDA4NP

C(1)-C(2)	1.378(2)	C(2)-C(1)-C(6)	120.85(12)
C(1)-C(6)	1.379(2)	C(2)-C(1)-N(1)	119.44(14)
C(1)-N(1)	1.4389(17)	C(6)-C(1)-N(1)	119.71(13)
C(2)-C(3)	1.3736(19)	C(3)-C(2)-C(1)	119.55(13)
C(3)-C(4)	1.399(2)	C(2)-C(3)-C(4)	121.19(12)
C(4)-O(3)	1.3090(15)	O(3)-C(4)-C(3)	122.57(12)
C(4)-C(5)	1.4026(19)	O(3)-C(4)-C(5)	119.91(12)
C(5)-C(6)	1.3695(19)	C(3)-C(4)-C(5)	117.52(12)
C(7)-N(2)	1.4698(18)	C(6)-C(5)-C(4)	121.33(13)
C(8)-N(2)	1.4811(16)	C(5)-C(6)-C(1)	119.52(13)
C(8)-C(8)$^{\#1}$	1.512(2)	N(2)-C(8)-C(8)$^{\#1}$	110.98(12)
C(9)-N(2)	1.4788(17)	O(1)-N(1)-O(2)	122.26(14)
N(1)-O(1)	1.222(2)	O(1)-N(1)-C(1)	118.54(14)
N(1)-O(2)	1.2242(19)	O(2)-N(1)-C(1)	119.20(15)
		C(7)-N(2)-C(9)	109.61(11)
		C(7)-N(2)-C(8)	113.18(11)
		C(9)-N(2)-C(8)	108.97(10)

Symmetry transformations used to generate equivalent atoms: #1 -x+2,-y,-z+2

Table S2 Hydrogen bonds for TMEDA4NP [Å and °]

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(2)-H(2A)...O(3)#2	0.953(9)	1.614(10)	2.5592(17)	170(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+2 #2 -x+3/2,y-1/2,-z+3/2

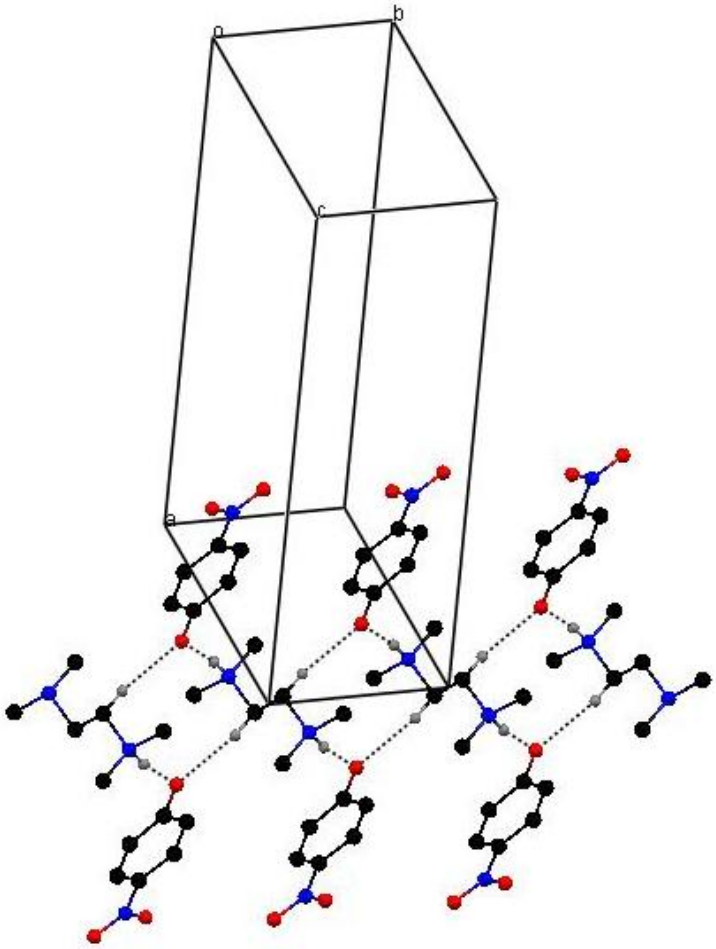

Fig. S1 View of hydrogen bonded network forming ring

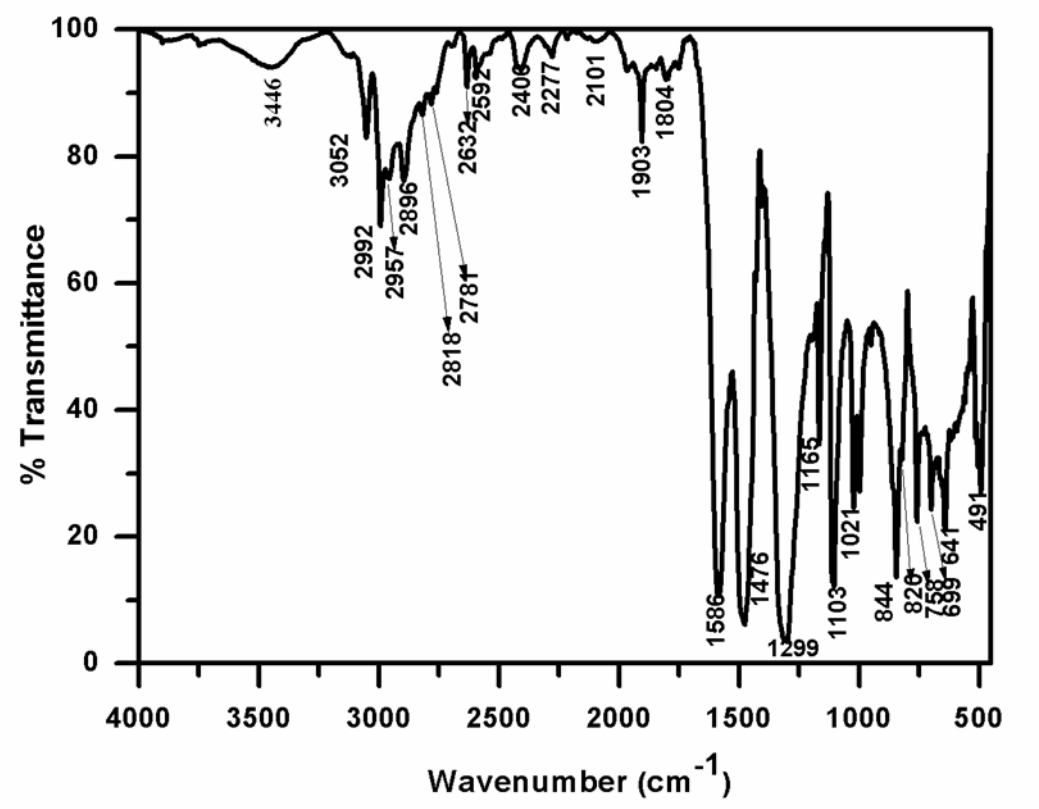

Fig. S2 FT IR Spectrum of TMEDA4NP

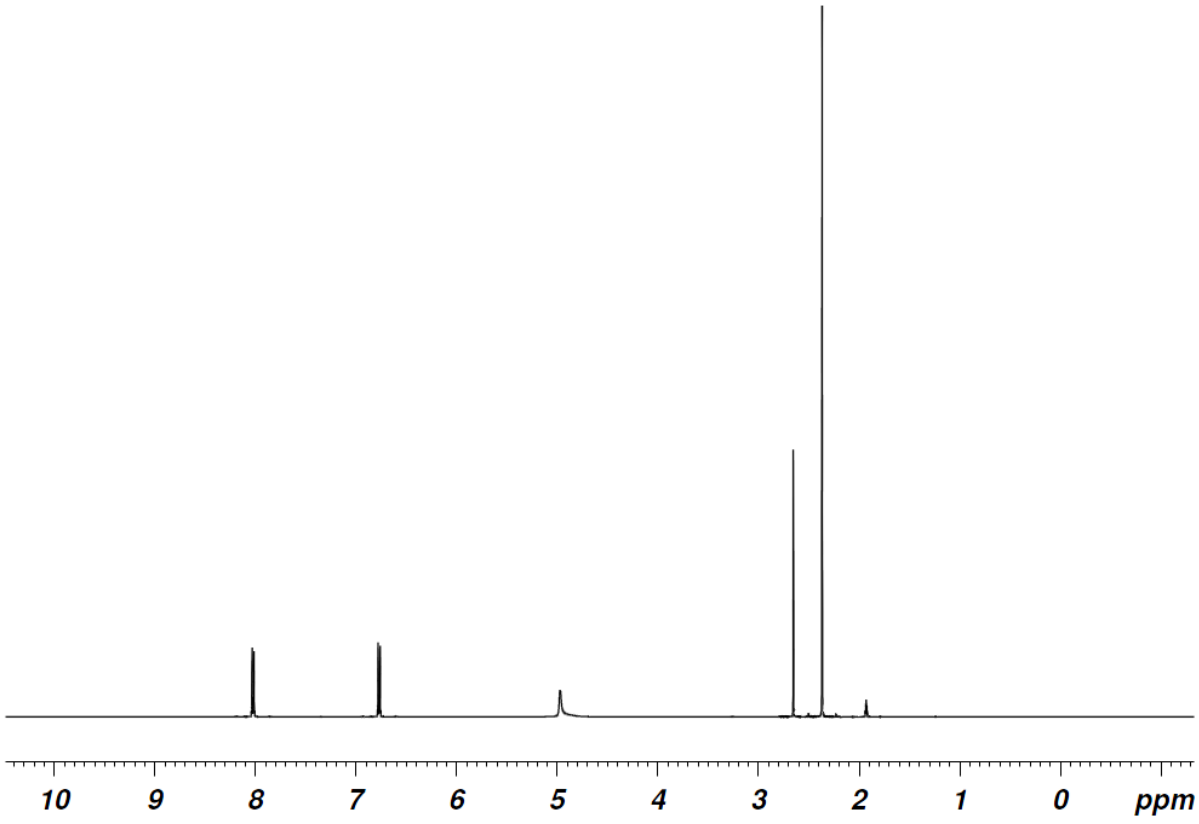

Fig. S3 500 MHz ^{1}H NMR spectrum of TMEDA4NP in CD_3CN at Room Temperature

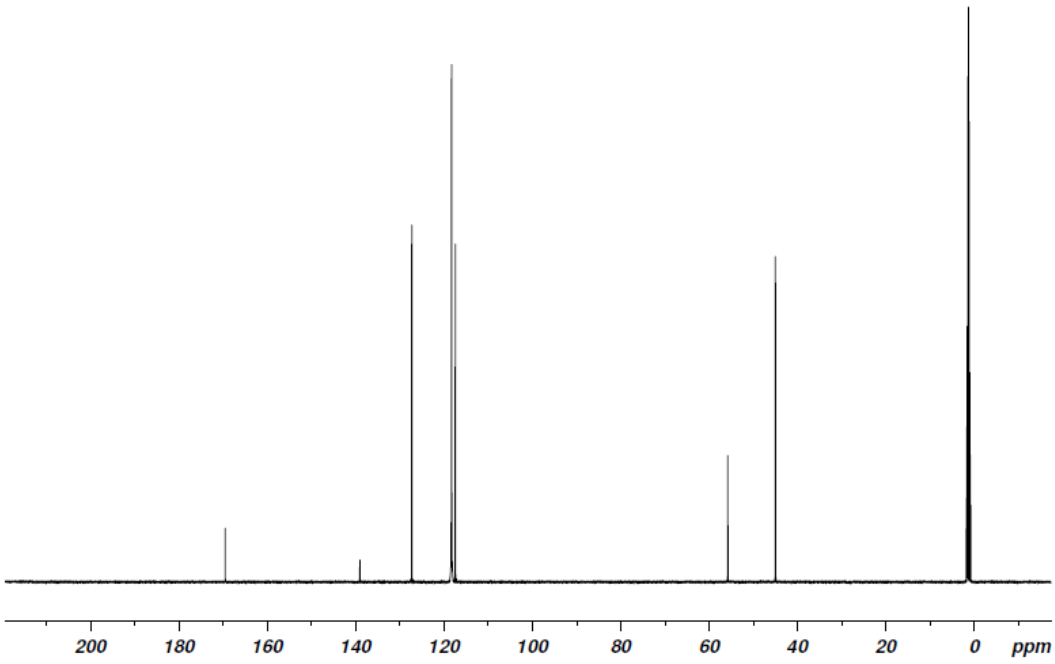

Fig. S4 ^{13}C NMR spectrum of TMEDA4NP in CD_3CN at Room Temperature

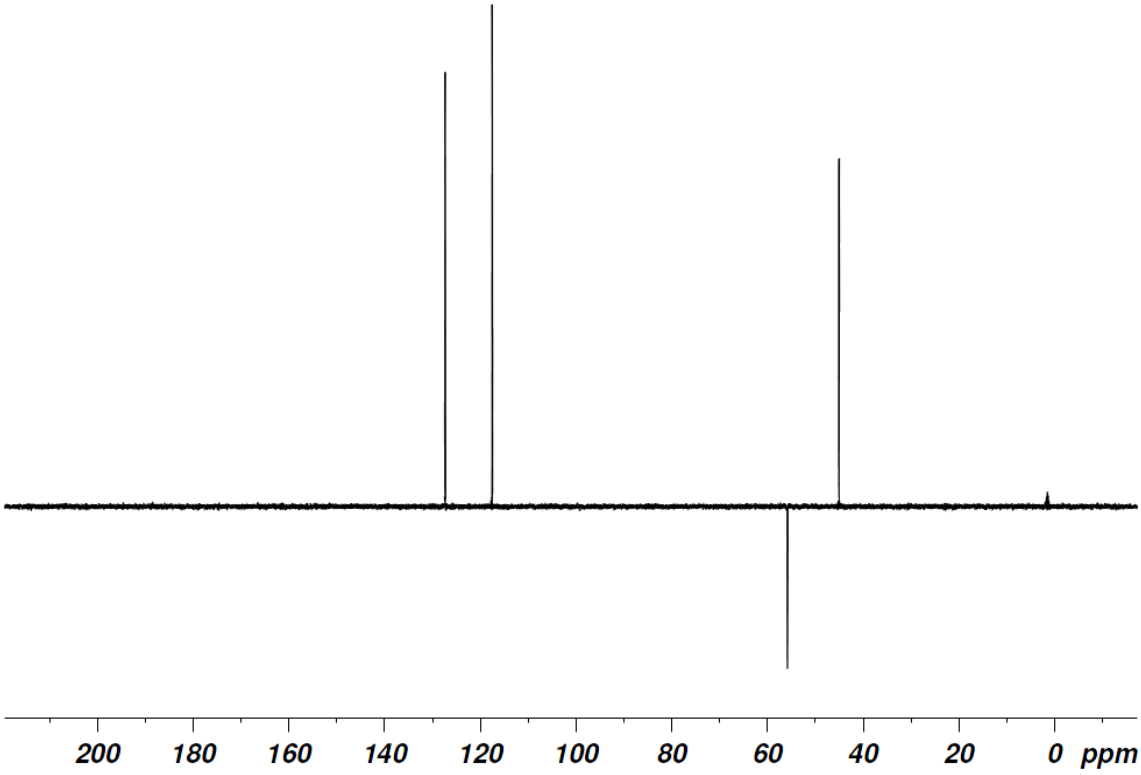

Fig. S5 DEPT-135 NMR spectrum of TMEDA4NP in CD_3CN at Room Temperature

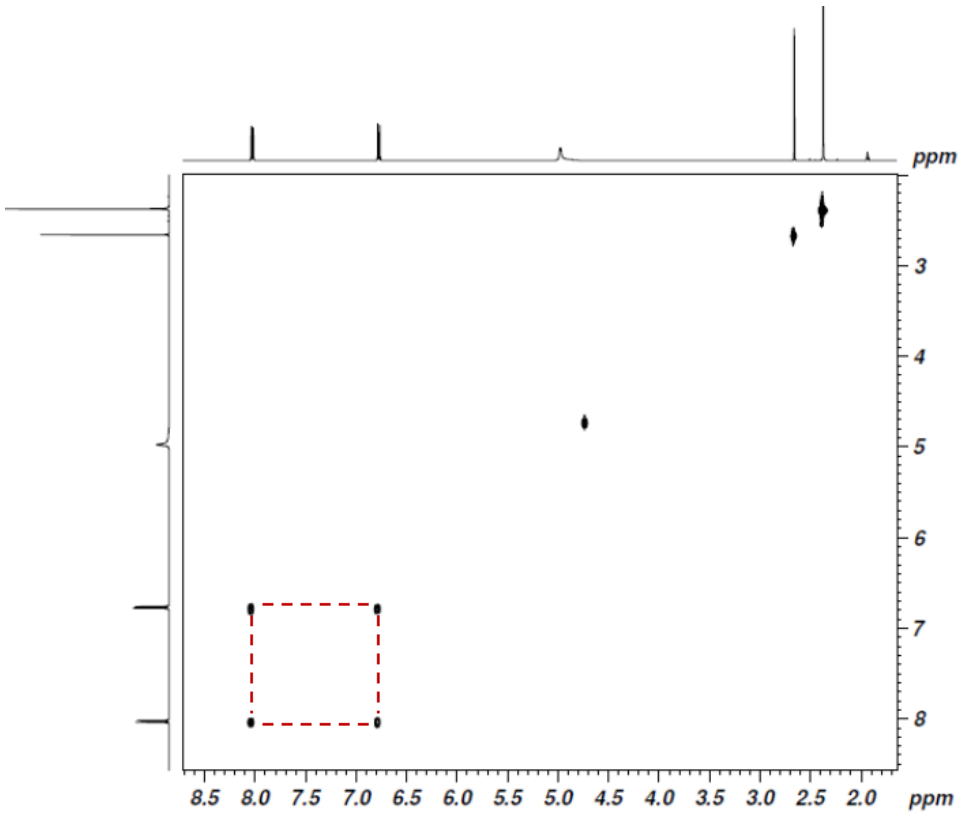

Fig. S6 COSY Spectrum of TMEDA4NP in CD_3CN

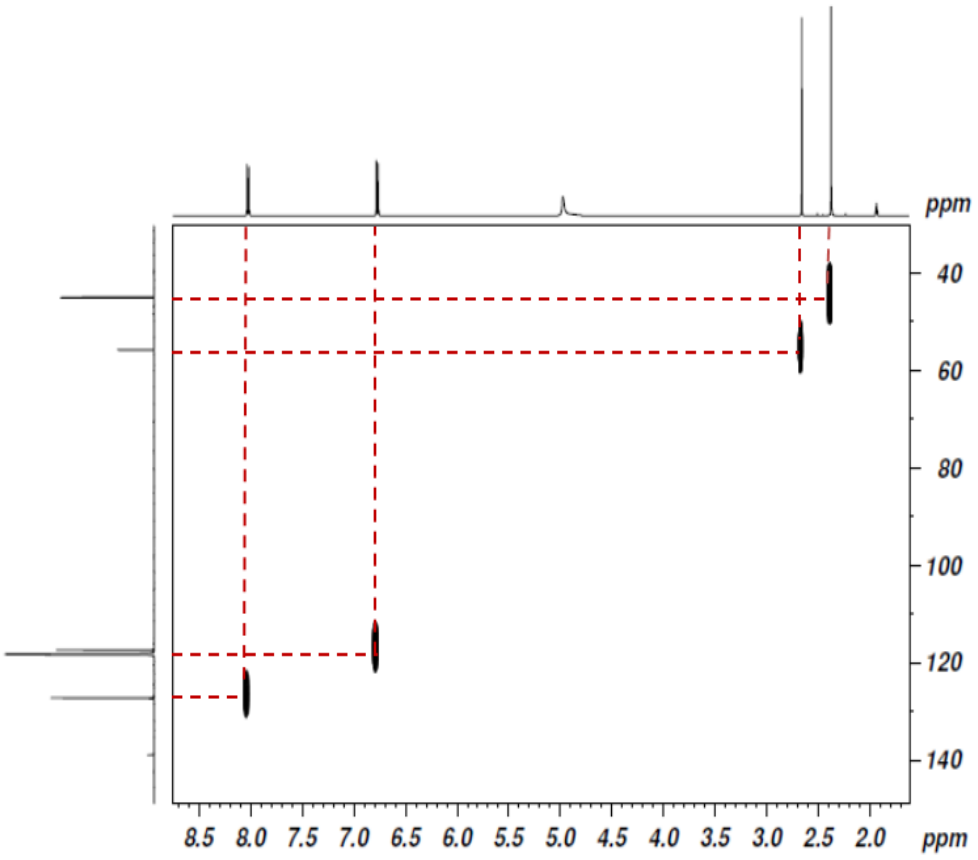

Fig. S7 HSQC spectrum of TMEDA4NP showing the one bond ^{1}H-^{13}C correlation