Electronic Supplementary Material (ESI) for New Journal of Chemistry.

ESI

Achieving AIE from ACQ in Positional Isomeric Triarylmethanes.

Soumya Singh, Abhineet Verma and Satyen Saha*
Department of Chemistry, Institute of Science, Banaras Hindu University, Varanasi - 221005

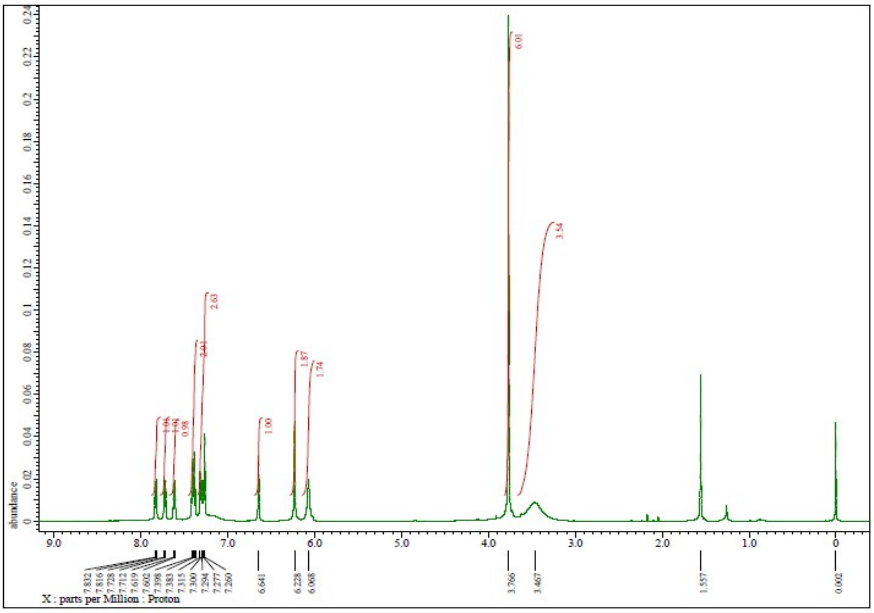

Figure S1(a). ^{1}H NMR spectra of AN in$CDCl_3$.

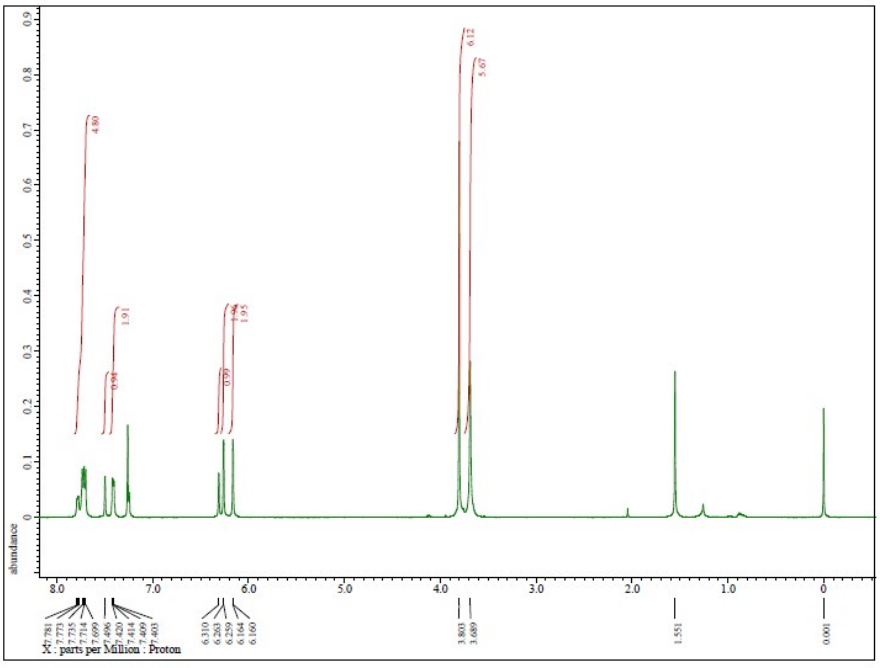

Figure S1(b). ^{1}H NMR spectra of BN in$CDCl_3$.

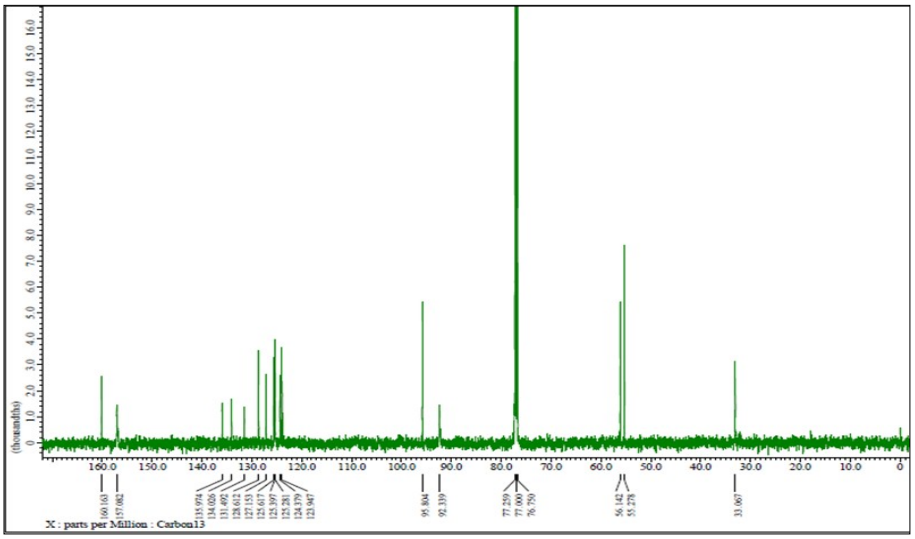

Figure S2(a). ^{13}C NMR spectra of AN in $CDCl_3$.

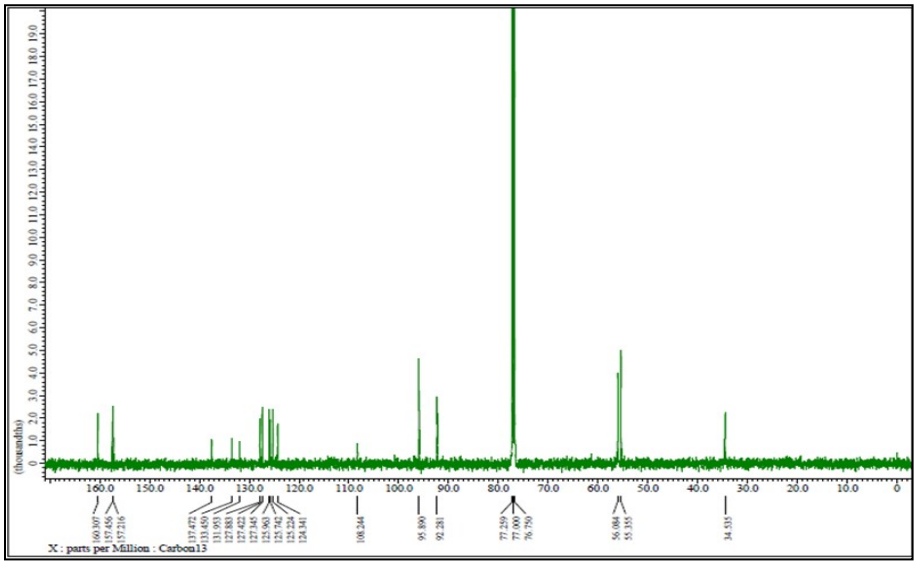

Figure S2(b). ^{13}C NMR spectra of BN in $CDCl_3$.

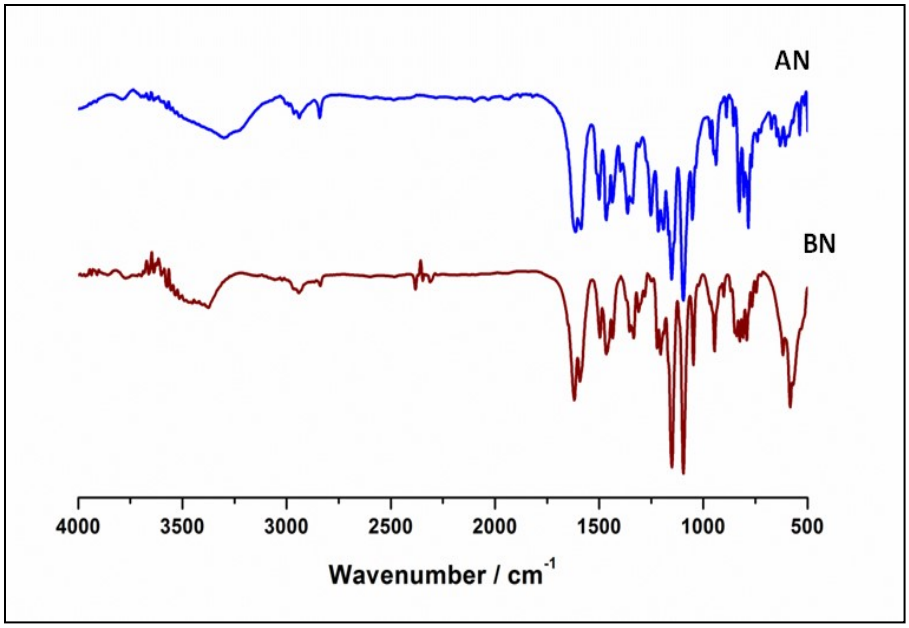

Figure S3. FT-IR of AN and BN.

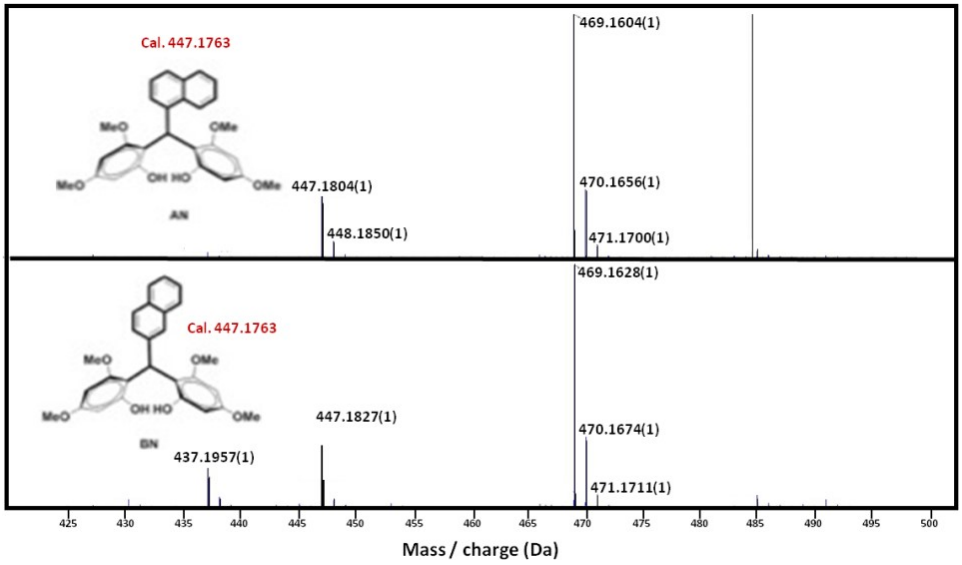

Figure S4. HRMS OF AN and BN.

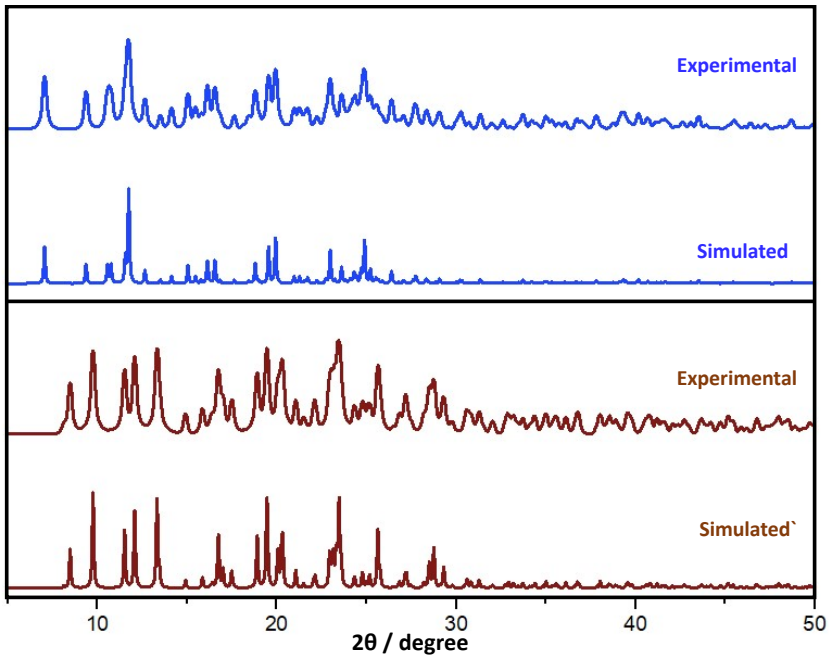

Figure S5. X ray powder diffraction of AN and BN.

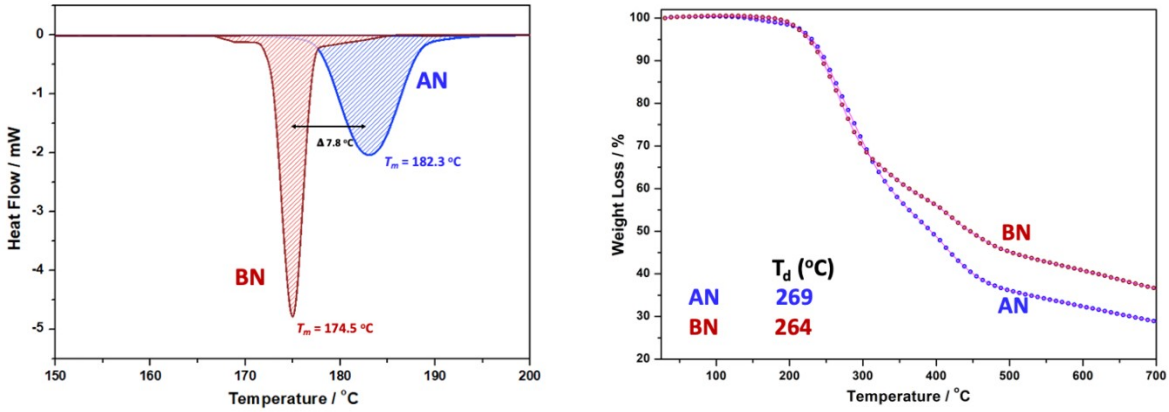

Figure S6. (a) TGA analysis for AN and BN. **(b)** DSC analysis of AN and BN.

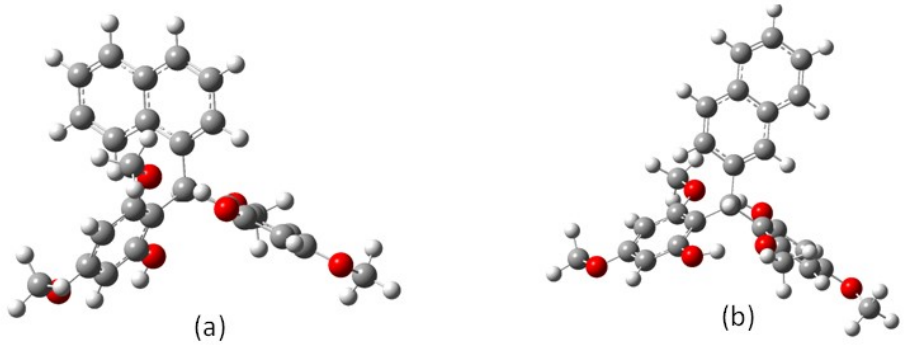

Figure S7. Optimized geometry of (a) AN (b) BN.

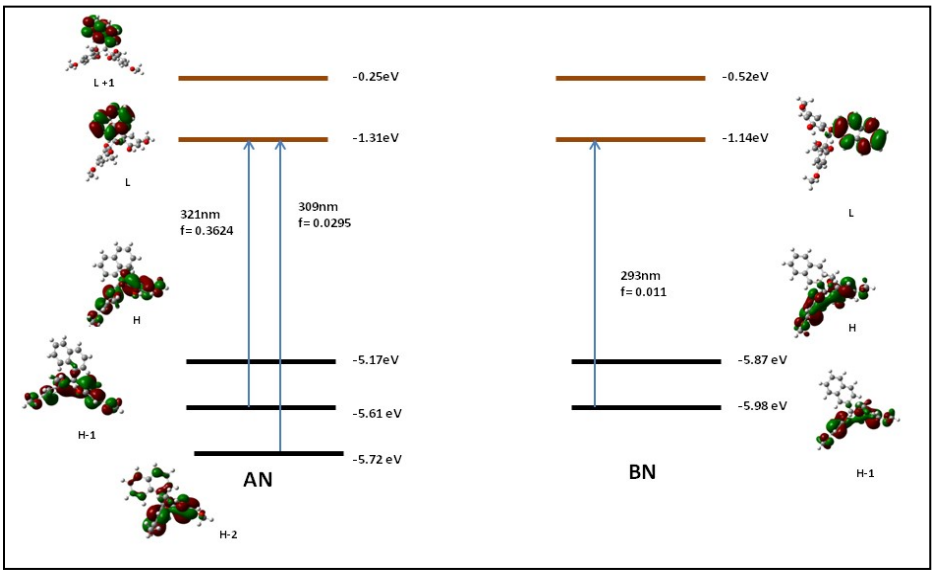

Figure S8. Molecular orbital diagram of AN and BN involved in electronic transition.

Table S1. Selected bond lengths (Å) and angles (°) for title complexes (**AN**).		
Bond length (Å)		
C12 C11 1.5256(5) O1 C13 1.3644(4) O2 C24 1.4189(4) O6 C21 1.3721(5) O3 C25 1.4335(4)	C11 C10 1.5231(5) O4 C19 1.3853(4) O5 C23 1.3701(4) O6 C27 1.4211(5)	C18 C11 1.5194(5) O2 C17 1.3898(3) O5 C26 1.4159(4) O3 C15 1.3569(5)
Angle (°)		
C12 C11 C18 112.95(3) C24 O2 C17 120.07(3) C12 C13 O1 115.30(3) C22 C23 O5 122.49(3) C14 C15 O3 115.14(2)	C10 C11 C18 114.75(2) C26 O5 C23 118.36(3) C14 C13 O1 121.37(2) C20 C21 O6 115.45(2) C16 C15 O3 125.09(3)	C10 C11 C12 116.63(3) C27 O6 C21 117.19(2) C18 C23 O5 114.74(3) C22 C21 O6 123.84(3)

Table S2. Selected bond lengths (Å) and angles (°) for title complexes (**BN**)		
Bond length (Å)		
C12 C11 1.5256(5) O1 C13 1.3644(4) O2 C24 1.4189(4) O6 C21 1.3721(5) O3 C25 1.4335(4)	C11 C10 1.5231(5) O4 C19 1.3853(4) O5 C23 1.3701(4) O6 C27 1.4211(5)	C18 C11 1.5194(5) O2 C17 1.3898(3) O5 C26 1.4159(4) O3 C15 1.3569(5)
Angle (°)		
C12 C11 C18 112.95(3) C24 O2 C17 120.07(3) C12 C13 O1 115.30(3) C22 C23 O5 122.49(3) C14 C15 O3 115.14(2)	C10 C11 C18 114.75(2) C26 O5 C23 118.36(3) C14 C13 O1 121.37(2) C20 C21 O6 115.45(2) C16 C15 O3 125.09(3)	C10 C11 C12 116.63(3) C27 O6 C21 117.19(2) C18 C23 O5 114.74(3) C22 C21 O6 123.84(3)

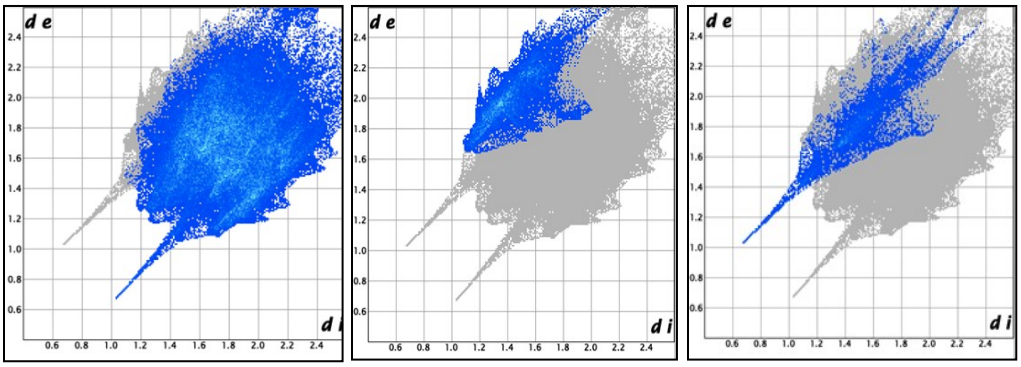

Fig S9 (a)- Relative surface area corresponding to each interaction for AN (i) H (ii) C (iii) O with others.

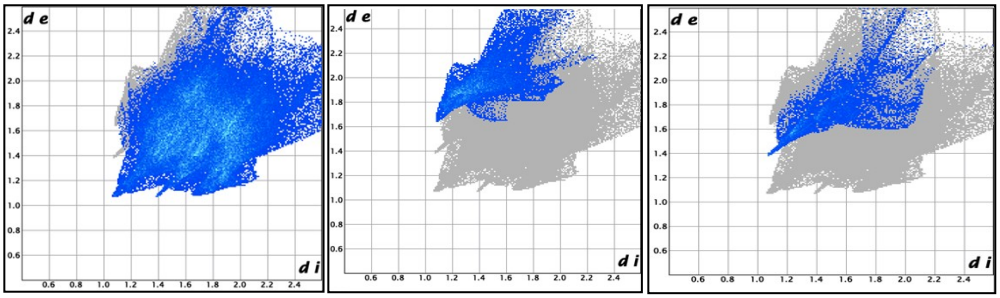

Figure S9 (b). Relative surface area corresponding to each interaction for BN (i) H (ii) C (iii) O with others.

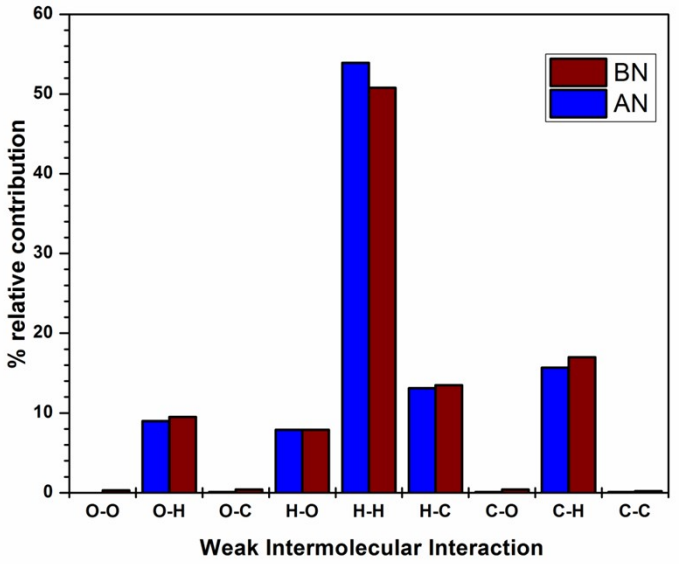

Figure S10. Relative percentage contribution of various intermolecular interaction.

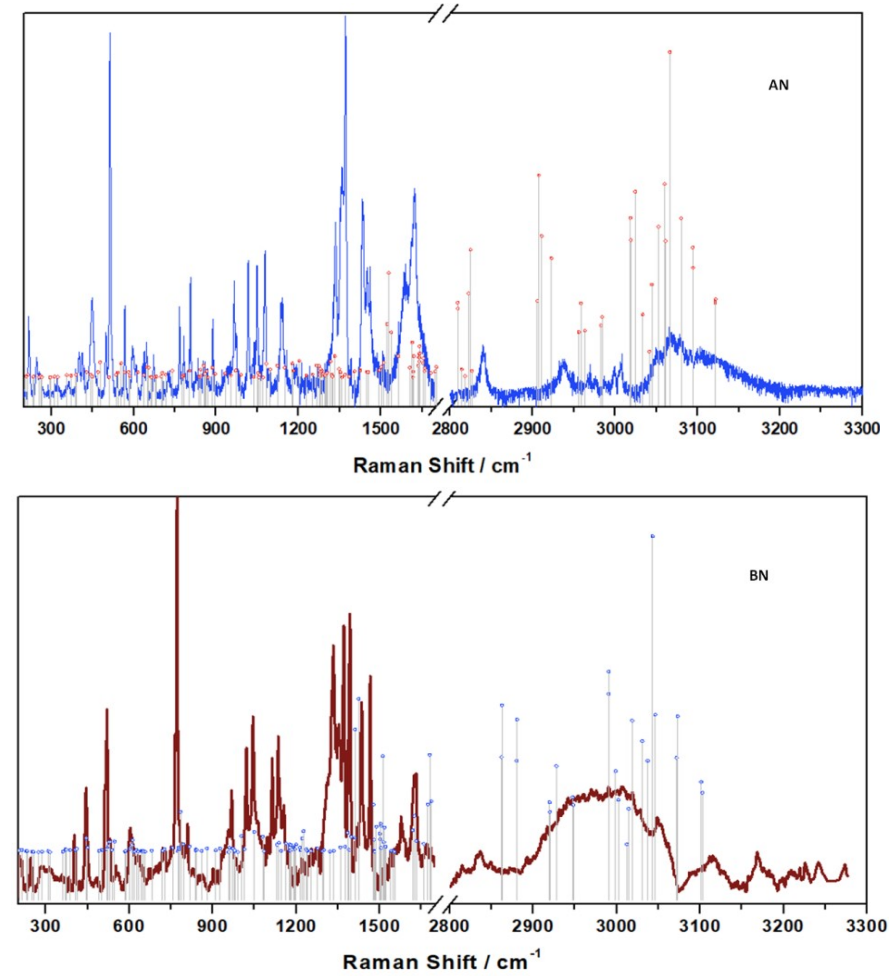

Figure S11. Raman Spetra of AN and BN.

Table S3. Calculated vibrational frequencies for AN and BN. A scaling factor of 0.960 is used on calculated frequencies. The possible assignments of vibration to the frequencies are done by observing the motion in GaussView.			
S.No.	**AN**	**BN**	**Assignment**
1.	246.8	246.2	Twisting vibrational modes
2.	400.8	401.9	Mixed vibrations
3.	449.8	444.2	Mixed vibrations
4.	515.6	519.7	Ring breathing vibrations
5.	600.6	603.1	Mixed twisting vibrations
6.	767.6	771.2	Methoxy ring hydrogen wagging mode
7.	807.4	803.4	Mixed ring breathing modes
8.	967.0	967.9	Ring breathing vibrations of methoxy moiety
9.	1049.0	1044.7	Naphthalene ring twisting vibrations
10.	1142.1	1135.7	Ring twisting vibrations
11.	1333.5	1333.5	-OH wagging coupled with ring breathing
12.	1371.2	1371.2	Methoxy moiety ring breathing vibrations
13.	-	1393.4	Mixed ring breathing vibrations
14.	1433.3	1436.2	Naphthalene hydrogen wagging vibrations
15.	1460.9	1466.6	Methoxy hydrogen twisting vibrations
16.	1620.2	1632.2	Ring breathing vibrations of naphthalene moiety
17.	2839.2	2837.1	C-H symmetric stretching
18.	2936.5	2948.3	C-H symmetric stretching
19.	3008.4	3010.3	C-H asymmetric stretching
20.	3067.4	3068.5	C-H asymmetric stretching

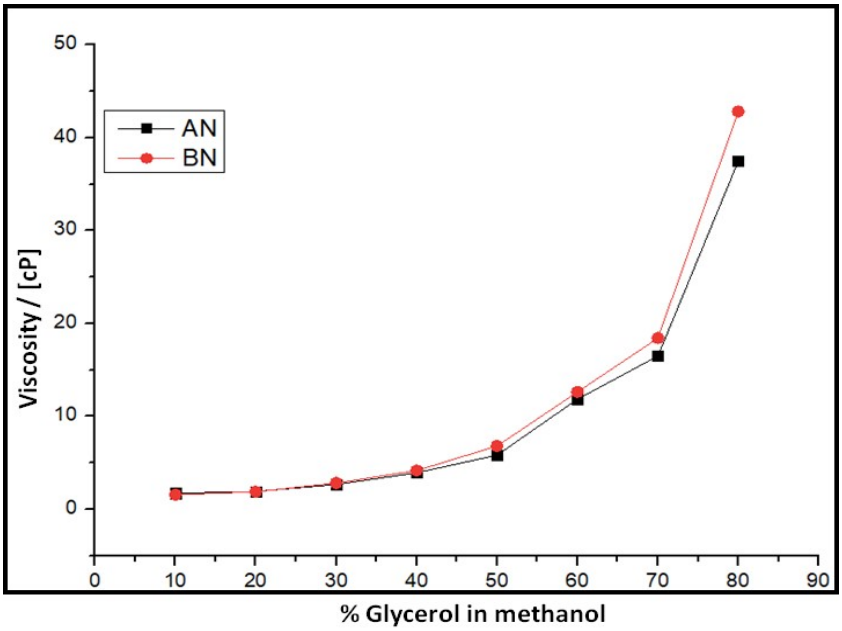

Figure S12. Viscosity change of **AN** and **BN** in Methanol glycerol mixture.

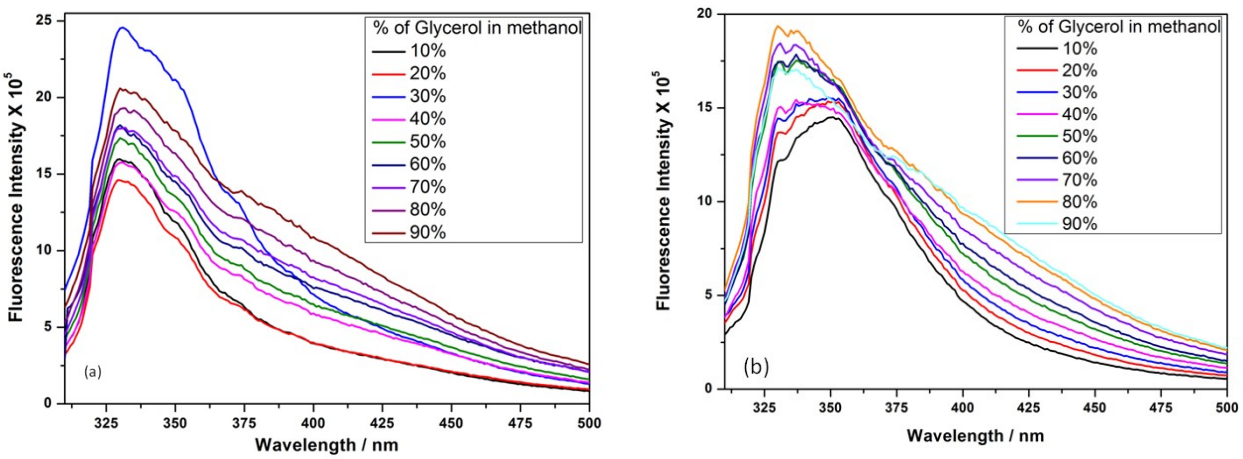

Figure S13. Emission spectra of (a) AN and (b) BN in methanol-glycerol mixture with increasing percentage of glycerol. While in both cases an increase of fluorescence intensities are observed, additional feature of blue shift can be observed only for BN.

Table S4. Antimicrobial activity Zone of inhibition (in mm).			
Compounds	Candida albicans	S.aureus (ATCC-25925)	E.Coli (ATCC-25922)
AN	6.5	6.5	6.5
BN	6.5	6.5	6.5

MIC (μg/ml)

Compounds	Candida albicans	S.aureus (ATCC-25925)	E.Coli (ATCC-25922)
AN	0.028	0.028	0.028
BN	0.028	0.028	0.028