

Supplementary Information

Remarkable dielectric properties of 1:2 inter-molecular compound of 2-(4-(Dimethylamino) benzylideneamino) benzoic acid and urea due to the excited-state intramolecular proton transfer

U.S. Rai*, Manjeet Singh, R. N. Rai

Department of Chemistry and Centre of Advanced Study, Institute of Science, Banaras Hindu University,
Varanasi- 221005, India

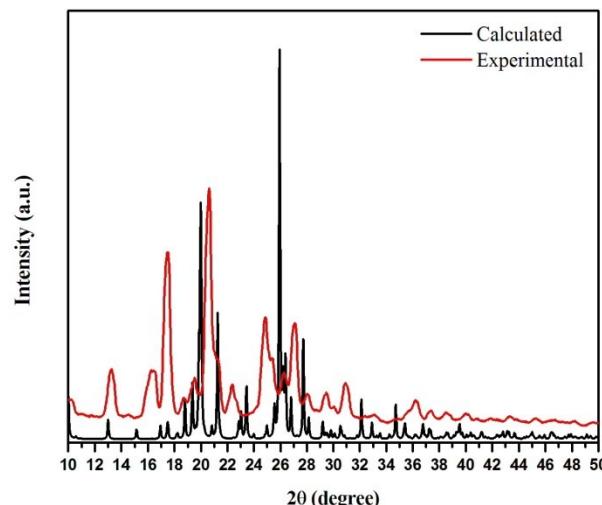


Figure S1: Comparison of calculated and experimental powder X-ray pattern of IMC

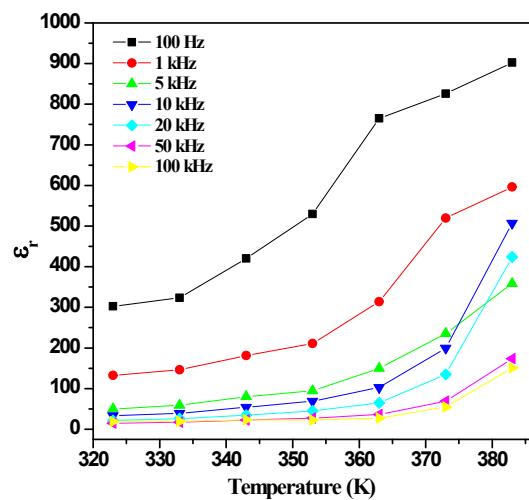


Figure S2: Variation of DEC with temperature at particular frequency

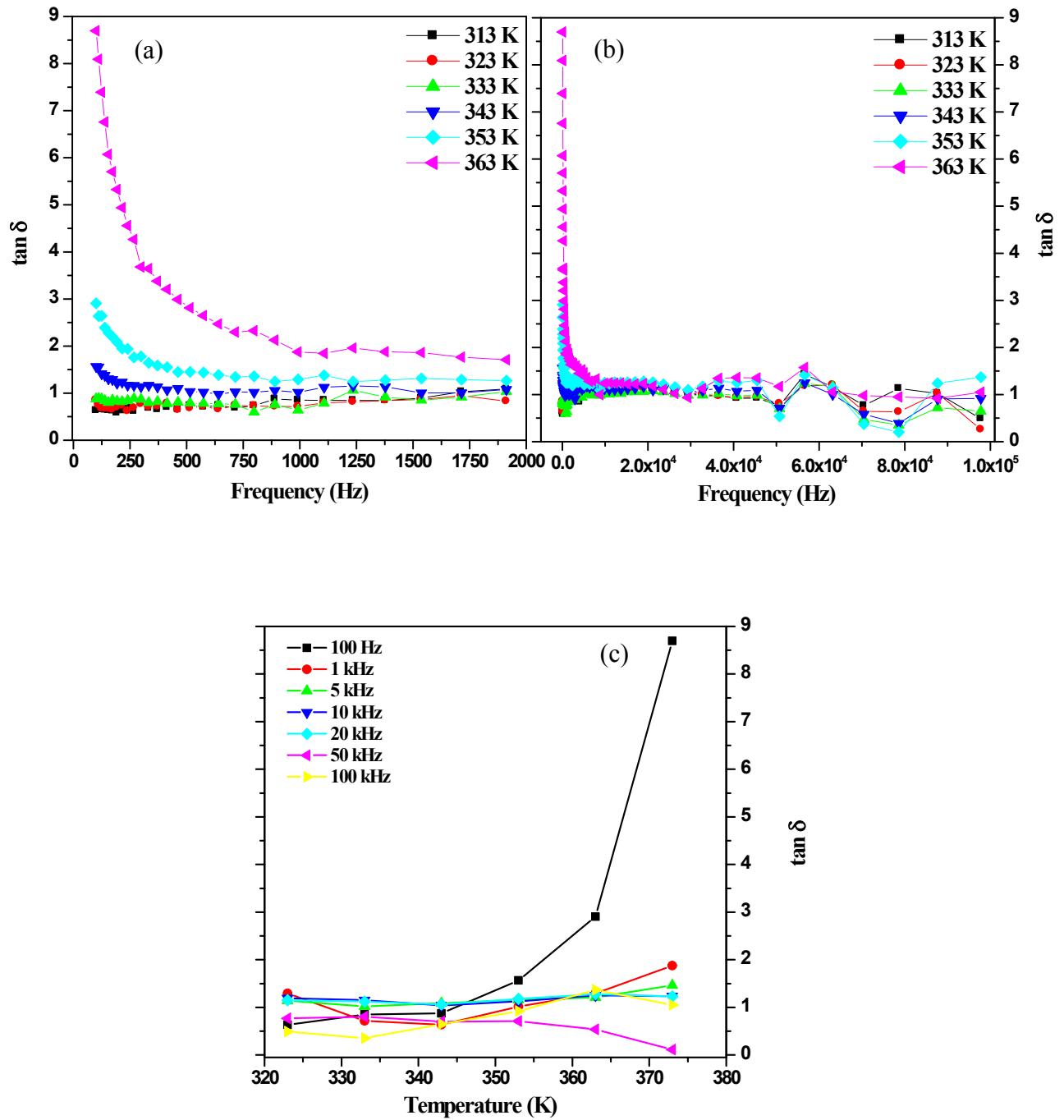


Figure S3: (a) and (b) Variation of dielectric loss of IMC with frequency at particular temperature and (c) Variation with temperature at particular frequency

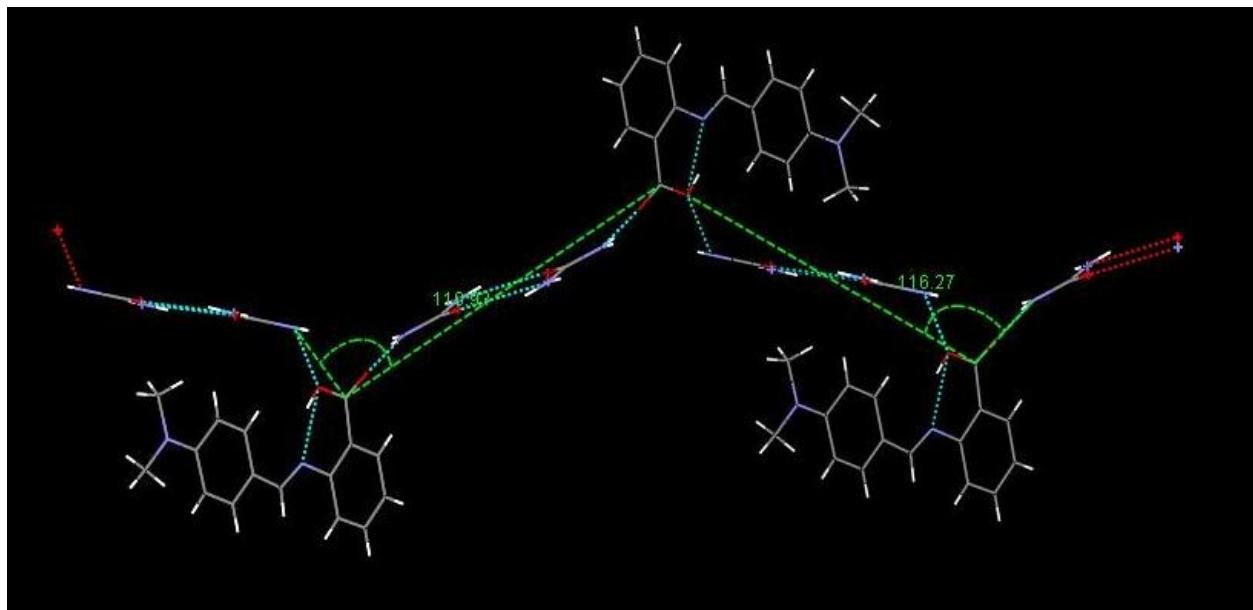


Figure S4: The angles between the polar nanodomains regions between DMABAB and U molecules

Table S1: Bond distances [\AA] and angles [$^\circ$] in the DMABAB-U IMC.

O4- C17	1.237(3)	O3- C18	1.235(3)	O2- C7	1.263(3)
N1- C8	1.310(3)	N1- C1	1.413(3)	C12- N2	1.341(3)
C12- C11	1.418(3)	C12- C13	1.431(3)	O1- C7	1.222(3)
N5- C18	1.338(3)	N2- C15	1.460(3)	N2- C16	1.461(3)
N3- C17	1.336(3)	C6- C5	1.383(3)	C6- C1	1.390(3)
C6- C7	1.532(4)	N6- C18	1.344(3)	N4- C17	1.358(3)
C10- C11	1.355(3)	C10- C9	1.405(3)	C9- C8	1.399(3)
C9- C14	1.429(3)	C14- C13	1.338(3)	C1- C2	1.414(4)
C2- C3	1.356(4)	C4- C5	1.382(4)	C4- C3	1.386(4)

C8- N1- C1	127.1(2)	N2- C12- C11	121.4(2)	N2- C12-13	121.5(2)
C11-C12-C13	117.1(2)	C12- N2- C15	121.6(2)	C12- N2-16	122.4(2)
C15- N2-C16	116.1(2)	C5- C6- C1	118.3(2)	C5- C6- C7	118.0(2)
C1- C6- C7	123.7(2)	O4- C17- N3	122.4(2)	O4- C17- N4	120.1(2)
N3- C17- N4	117.5(2)	C11- C10- C9	122.2(2)	C8- C9- C10	119.7(2)
C8- C9- C14	123.6(2)	C10- C9- C14	116.7(2)	C13- C14-C9	121.9(2)
N1- C8- C9	125.5(2)	C10- C11-C12	121.0(2)	C6- C1- N1	117.3(2)
C6- C1- C2	120.3(2)	N1- C1- C2	122.4(2)	C14-C13-C12	121.1(2)
O1- C7- O2	122.9(3)	O1- C7- C6	119.3(2)	O2- C7- C6	117.8(2)
O3 C18 N5	122.2(2)	O3 C18 N6	120.9(2)	N5- C18- N6	116.9(2)
C3- C2- C1	119.4(3)	C5- C4- C3	118.9(3)	C2- C3- C4	121.3(3)
C4- C5- C6	121.8(3)				