Electronic Supplementary Information

Evidence of CT Complex Formation Between Probe and Unreacted Methylimidazole in Imidazolium Cation Based Ionic Liquids: Sensing by Functionalised 2-Benzyledinemalononitrile

Manish Kumar Tiwari, Monika and Satyen Saha*

Department of Chemistry, Institute of Science, Banaras Hindu University,

Varanasi 221005, India. *E-mail:* satyen.saha@gmail.com

1. Literature published on different ionic liquids in recent years.

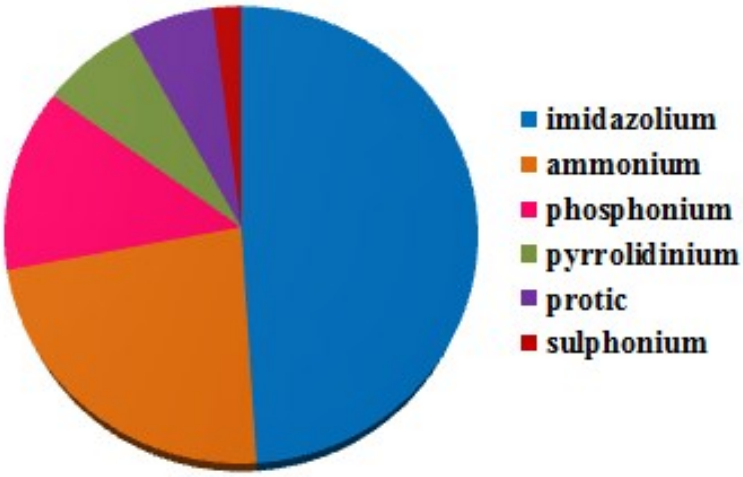


Fig.S-1: Papers published from 2010 to 2016 on different cation based ILs

2. Characteristic UV-Vis absorption bands of RDC in ACN

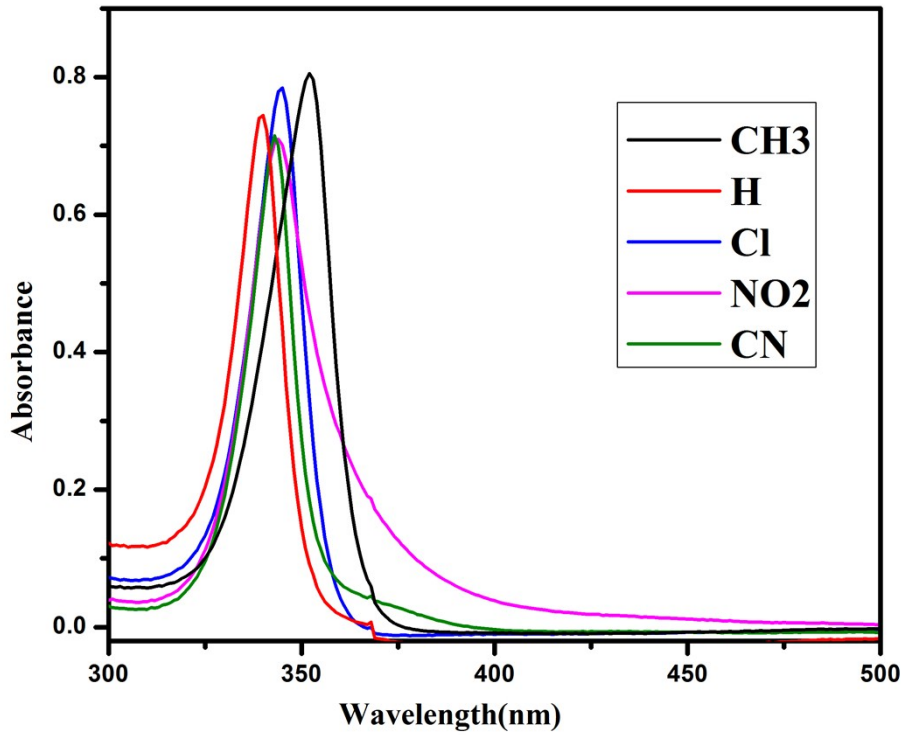


Fig. S-2: UV-Vis spectra of RDC in ACN.

3. Time dependent UV-Vis study of NDC in pure RTIL.

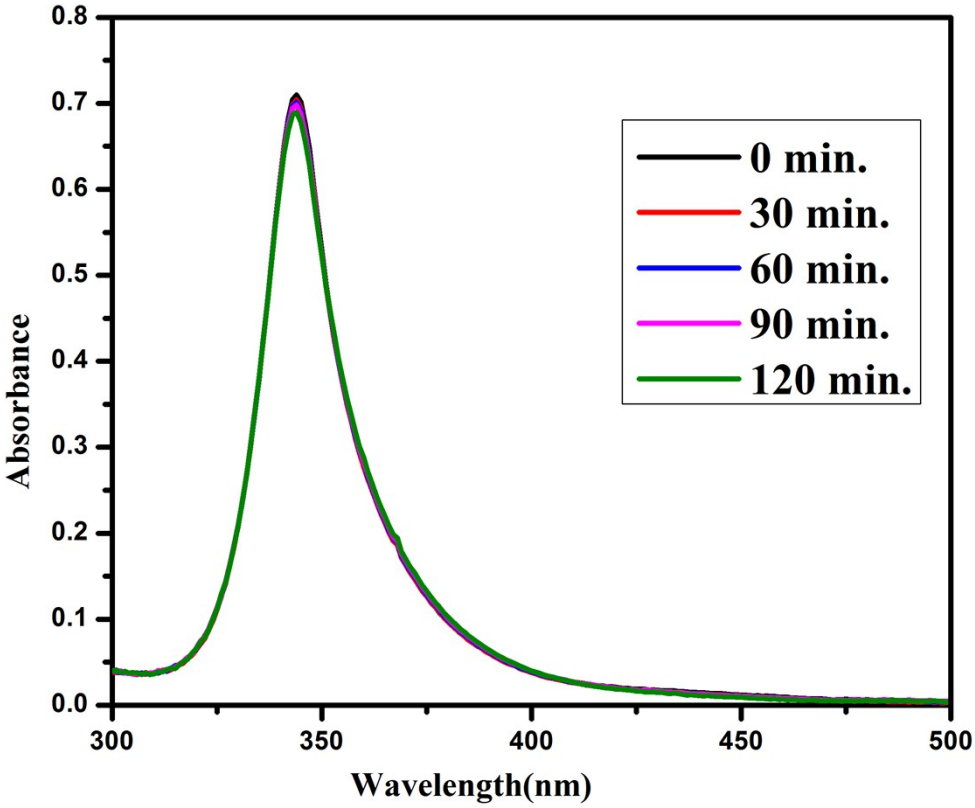


Fig. S-3: Time dependent UV-Vis spectra of NDC in pure bmimNTf$_2$ RTIL.

4. Time dependent UV-Visible study of NDC in different ionic liquids.

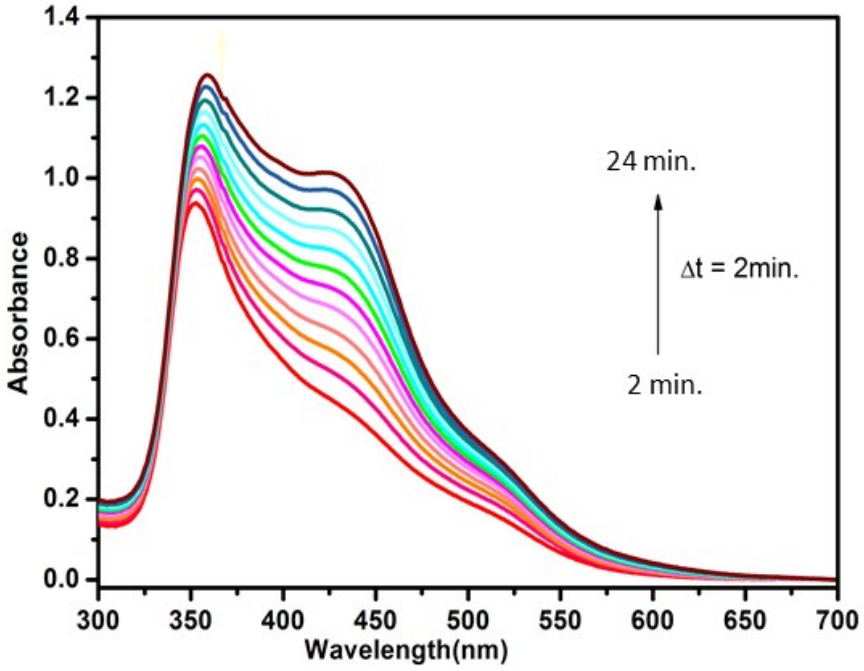


Fig. S-4 Time dependent UV-Vis spectra of the reaction of residual MIM with NDC in bmimCl.

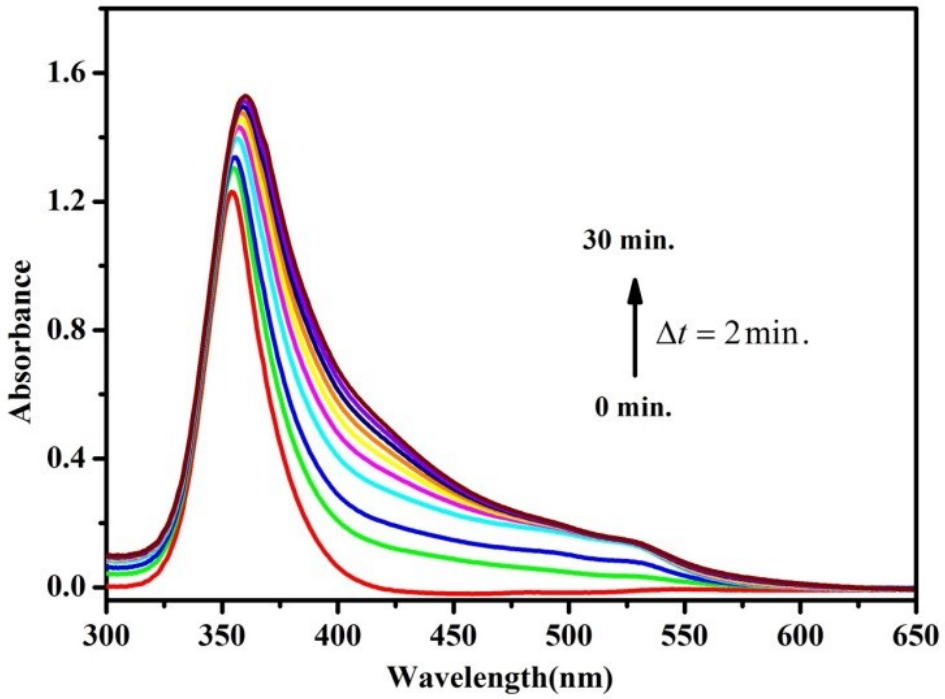


Fig.S-5: UV-Vis spectra of NDC in bmimPF_6 having 0.1 mole% of MIM at different time.

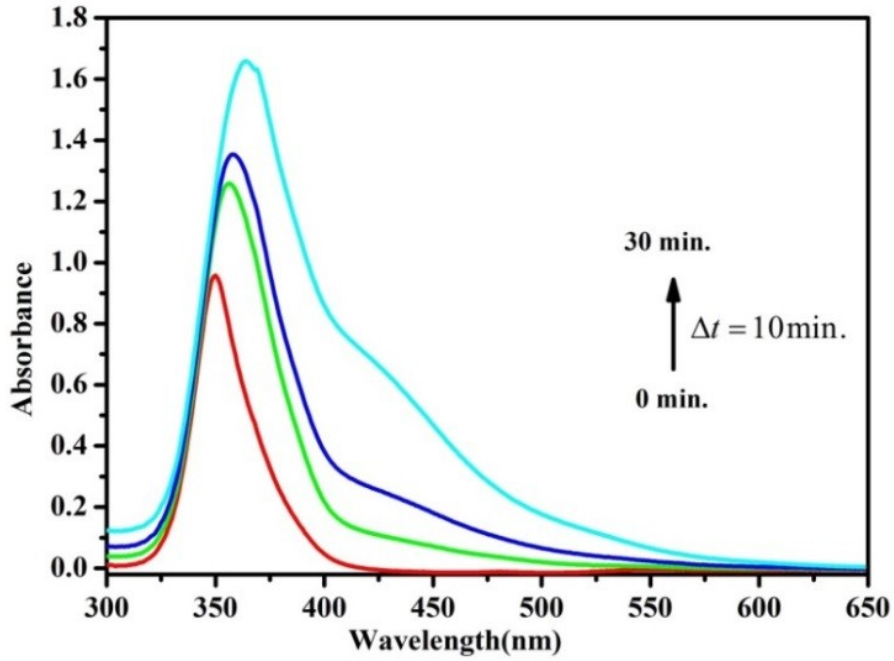


Fig.S-6: UV-Vis spectra of NDC in bmimNTf_2 having 0.2 mole% of MIM at different time.

5. Photometric titration

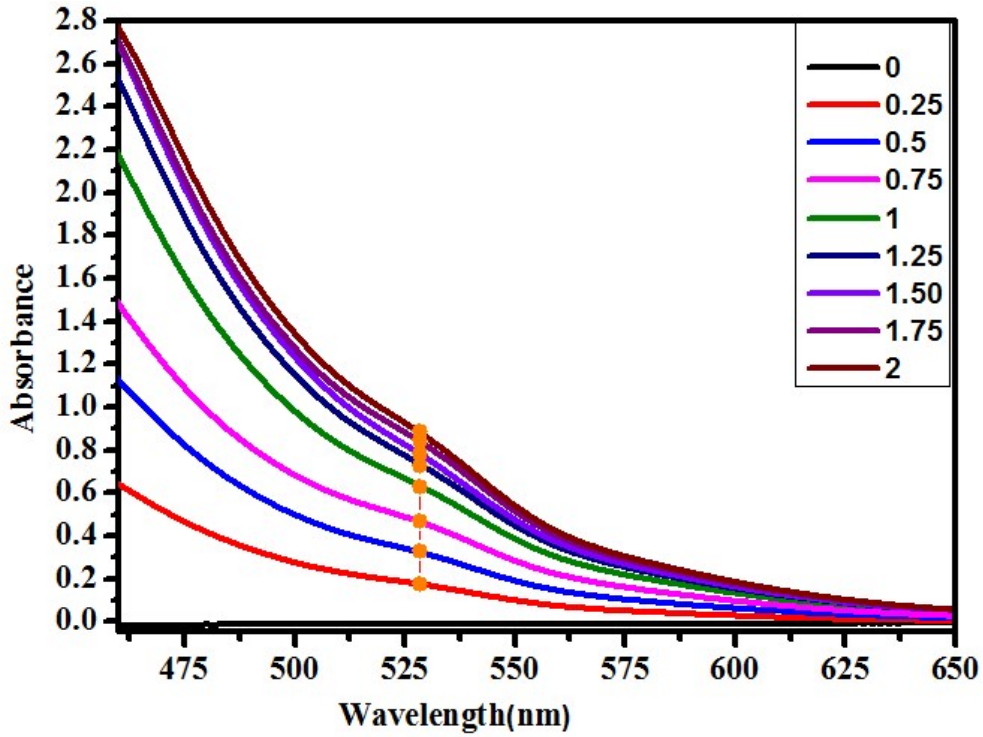
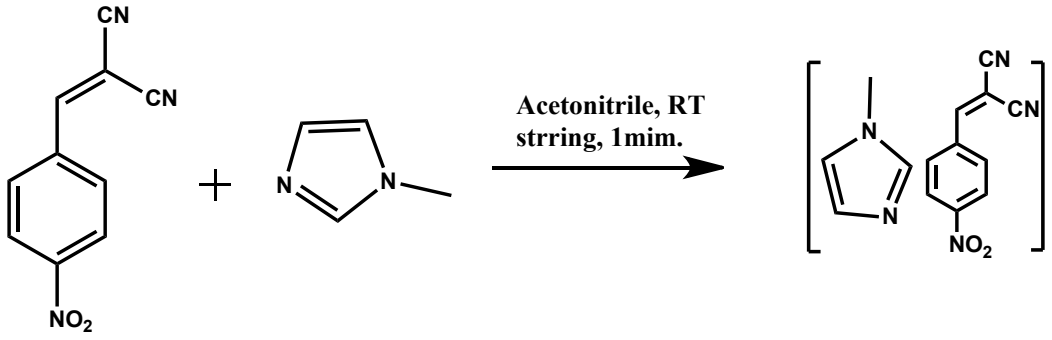


Fig. S-7: Formation of NDC-MIM charge transfer complex in ACN solvent. The absorption at 528nm is monitored and used for determination of stoichiometry of the complex. The amount of successive addition of NDC is shown in legend in a fixed concentration solution of MIM in ACN.

6. Formation of CT complex.



Scheme S-1. Schematic representation of formation of CT complex.

7. NMR Spectra

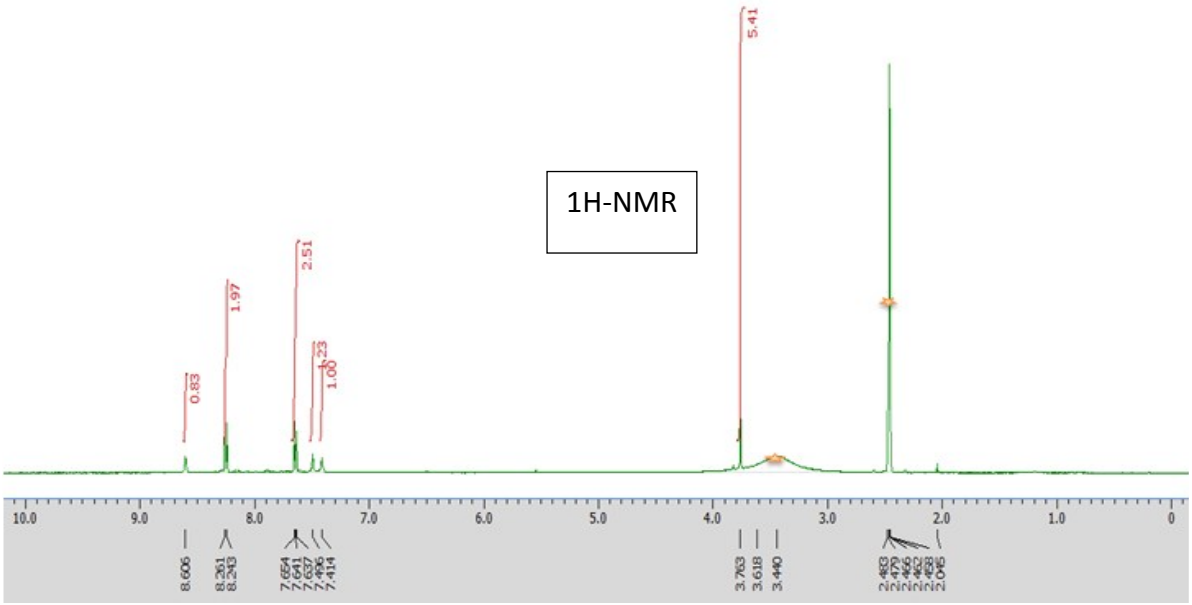


Fig.S-8: H-NMR spectrum of CT complex [NDC][MIM]

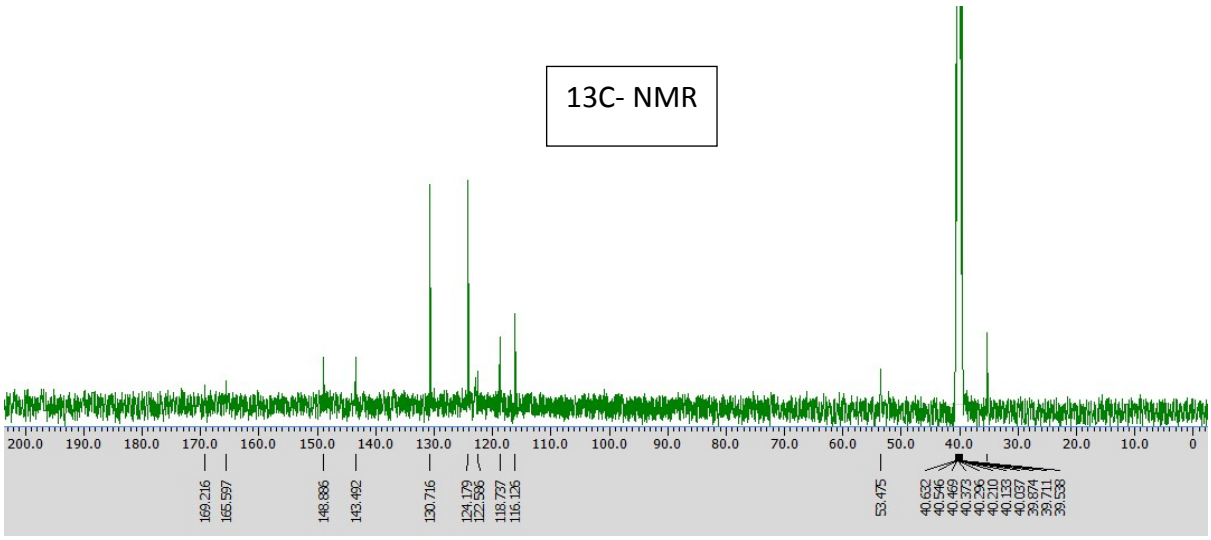


Fig.S-9: H-NMR and 13C NMR spectrum of CT complex [NDC][MIM]

Details of peak analysis of NMR:

1H NMR (500 MHz, DMSO-d6) δ (ppm) = 8.60 (s, 1H), 8.25(d, J =10 Hz, 2H), 7.64 (d, J = 10 Hz 2H), 7.63(s, 1H), 7.49 (s, 1H), 7.41 (s, 1H), 3.76 (s, 3H).);

13C NMR (125 MHz, DMSO-d6) δ (ppm) = 169.216, 165.597, 148.88, 143.49, 130.71, 124.17, 122.58, 118.73, 116.12, 53.47, 39.53.

8. FTIR

The infrared bands of the acceptor NDC and the CT complex [NDC-MIM] were shown in **Fig. S-3** in a comparative manner. CT complex contained all the peaks of NDC but in lower in intensity with noticeable shifts in the wavenumbers as compare to NDC. For example 1414cm-1 is shifted to 1476 cm-1 and 2231 cm-1 shifted to 2193 cm-1.

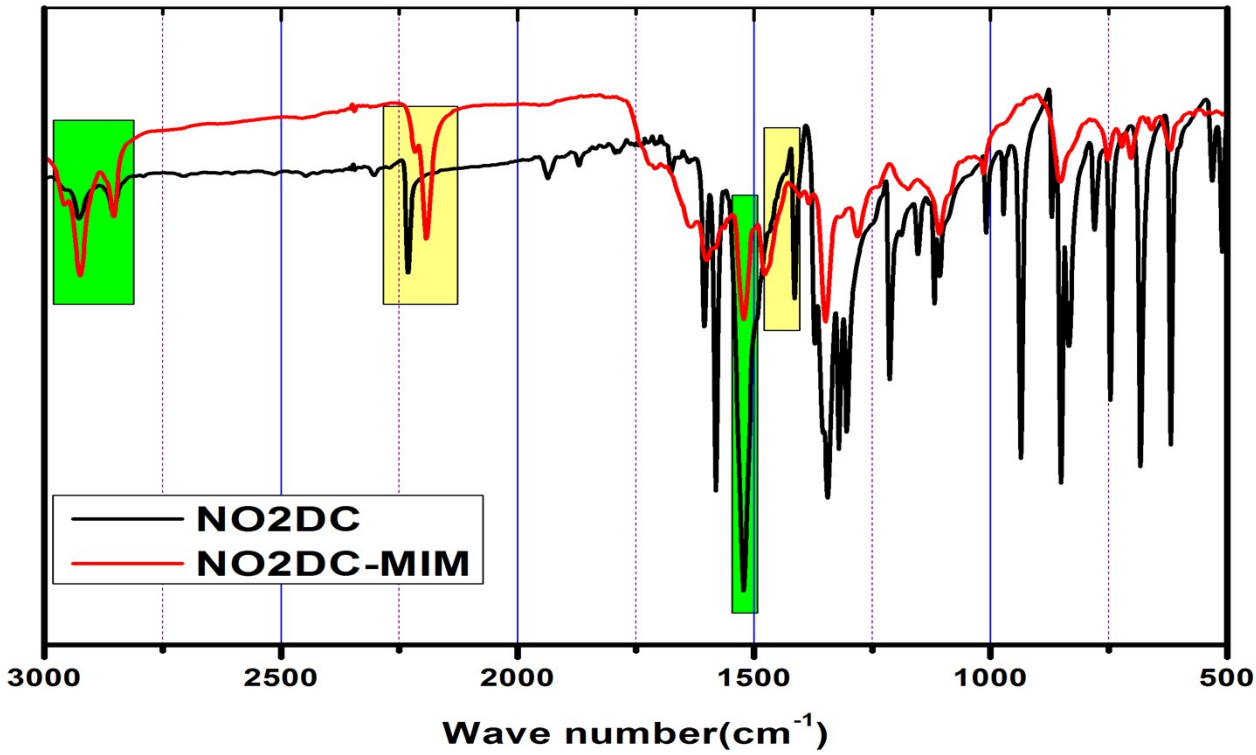


Fig.S-10: Comparative IR data of NDC and [NDC][MIM].

9. Minimum detection quantity of MIM through NDC.

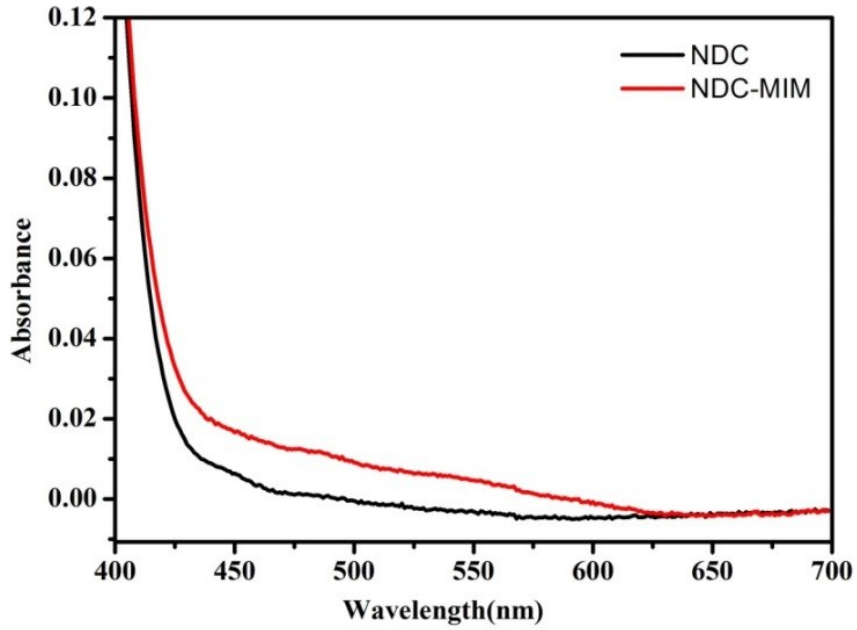


Fig S-11: UV-Vis spectra of NDC with .01 mole % MIM in bmimBF4