Supplementary Material

Molecular Dynamics and Translational-Rotational Coupling of an Ionically Conducting Glass-former: Amlodipine Besylate

Safna Hussan K.P.*[1], Mohamed Shahin Thayyil[1], S.K. Deshpande [2], Jinitha T.V.[3], Manoj K.[4], K.L. Ngai[5]

[1]*Department of Physics, University of Calicut, Malappuram-673635, Kerala, India*

[2] *UGC-DAE Consortium for Scientific Research, Mumbai Centre, BARC, Mumbai,40085, India*

[3]*Department of Chemistry, University of Calicut, Malappuram-673635, Kerala, India*

[4]*College of Pharmaceutical Sciences, Govt. Medical College, Kozhikode-673008, Kerala, India*

[5]CNR-IPCF, Largo Bruno Pontecorvo 3, I-56127, Pisa, Italy

Molecular Dynamics

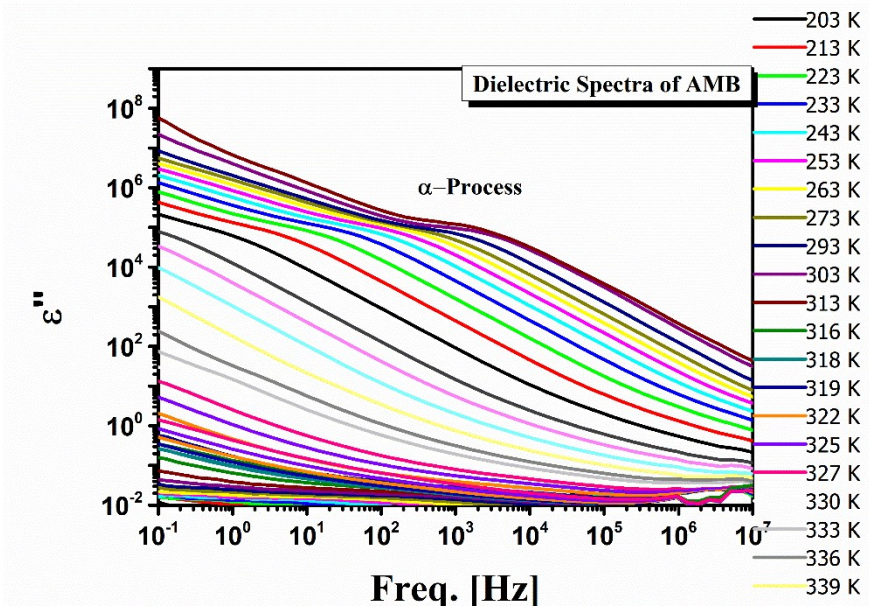

Fig S1: The dielectric loss of AMB over wide temperatures from the deep glassy to supercooled liquid states. Structural relaxations of AMB are masked by the conductivity.

We have measured the real ε′(f) and imaginary ε″(f) part of the complex dielectric response ε□(f)= ε′(f)-iε″(f) over a wide temperature range. The dielectric loss spectra of AMB were shown in **Fig.S1.** It was found that the dielectric loss spectra collected in the supercooled liquid state exhibits were dominated by dc-conductivity, associated with hopping of ions, especially the amlodipine cation and the besylate anion in AMB, making it

impossible to observe the structural relaxation in the dielectric susceptibility. Thus it is difficult to point out the structural α -relaxation times (τα) and to do further analysis with it.

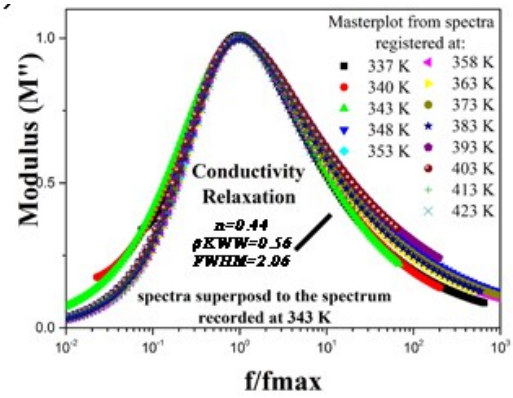

Fig S2: The master plot of AMB formed by horizontally shifting several spectra near T_g to overlap the spectra to 343 K

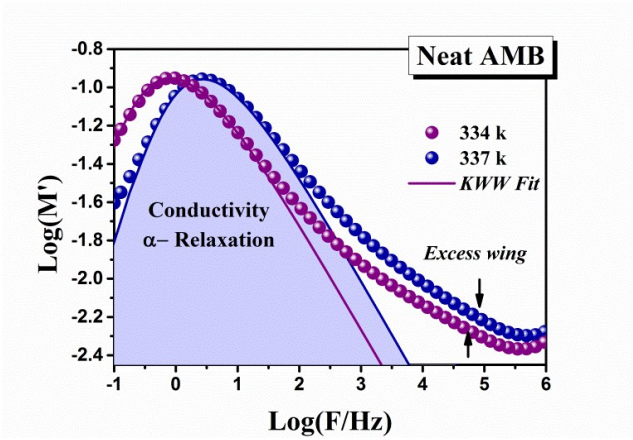

Fig S3: Shows the KWW fit at 334 K and 337K, especially temperature dependent excess wing.

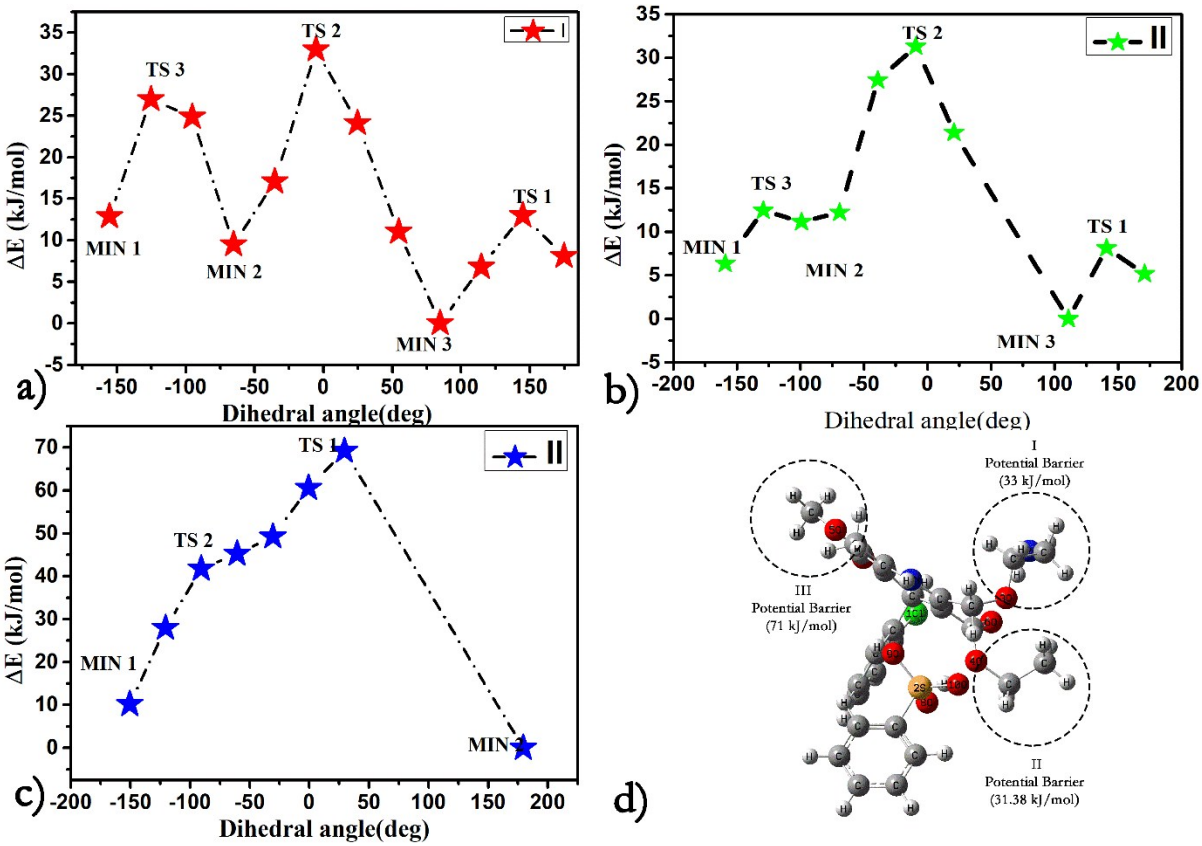

Fig S4. The diagram representing changes of energy during the rotation of all possible dihedral side chain in AMB. **a)** Around 30 atom **b)** around 4O atom **c)** around 5O atom **d)** Schematic diagram of rotated dihedral side chains in AMB molecule. MIN—minimum, TS—transition state (top)

In order not to exclude the occurrence of an intra-molecular secondary relaxation, we have pursued computer simulation studies of AMB molecule by incorporating all possible side-chain rotations about various dihedral angles. Among all of the dihedral side chains, the rotation around the third oxygen atom has barrier energy of 33 kJ/mol comparable to the experimental activation energy of 38.9 ± 0.05 kJ/mol for the secondary relaxation. The barrier energy corresponding to 4O is small while that of 50 is very much large.

The energy conformation is plotted for each dihedral angle are shown in Fig S4.