Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic supplementary information

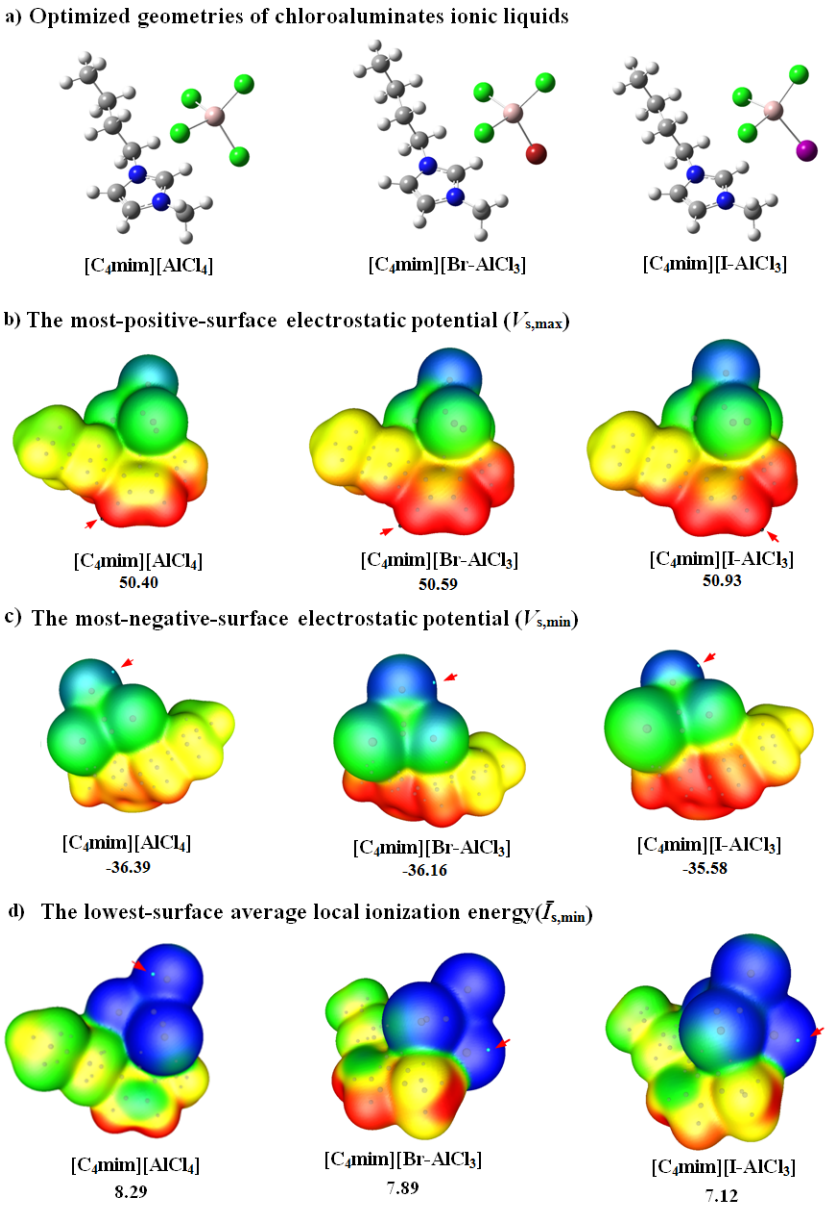

Fig. S1 (a) Optimized geometries of chloroaluminates ionic liquids at the B3LYP/aug-cc-pvdz level ; (b) electrostatic potential at the 0.001 au contour of the electron density and its maximum $V_{s,max}$ on the ILs; (c) electrostatic potential at the 0.001 au contour of the electron density and its minimum $V_{s,min}$ on the ILs; (d) average local ionization energy at the 0.001 au contour of the electron density and its minimum $\bar{I}_{s,min}$ on the ILs. Color ranges for electrostatic potential, in kcal/mol: blue < −30.0 < green < -4 < yellow < 20 < red. Color ranges for average local ionization energy, in eV: blue < 10 < green < 12 < yellow < 14 < red. The positions of $V_{s,m}$ and $\bar{I}_{s,min}$ are marked by the red arrow on the surface.

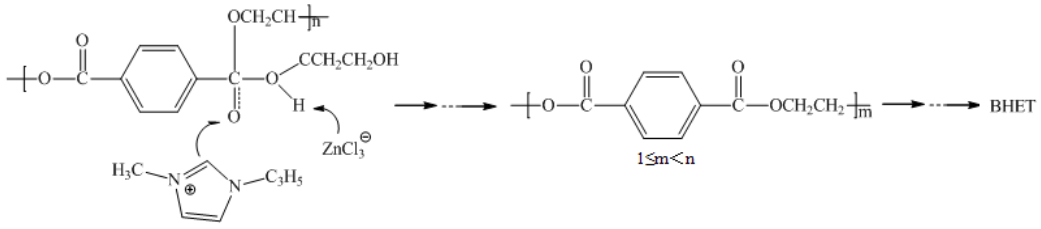

Fig. S2 The proposed mechanism for the degradation of PET catalyzed by [amim][$ZnCl_3$].