

Supplementary Information

Mixed-halide engineering in a homopiperazinium hybrid salt: structural disorder description, electronic structure analysis, and bioactivity evaluation

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The occupied orbitals HOMO-2 and HOMO-1 are predominantly localized on the organic homopiperazinium cation, particularly around nitrogen atoms and adjacent carbon chains, indicating their participation in electron-donor behavior. In contrast, the unoccupied orbitals LUMO+1 and LUMO+2 exhibit stronger localization on the bromide/chloride sublattice, confirming the electron-acceptor role of the mixed halide environment. The progressive orbital delocalization observed near the frontier region supports the presence of ligand-to-halide charge-transfer transitions and explains the UV-active optical behavior of the compound.

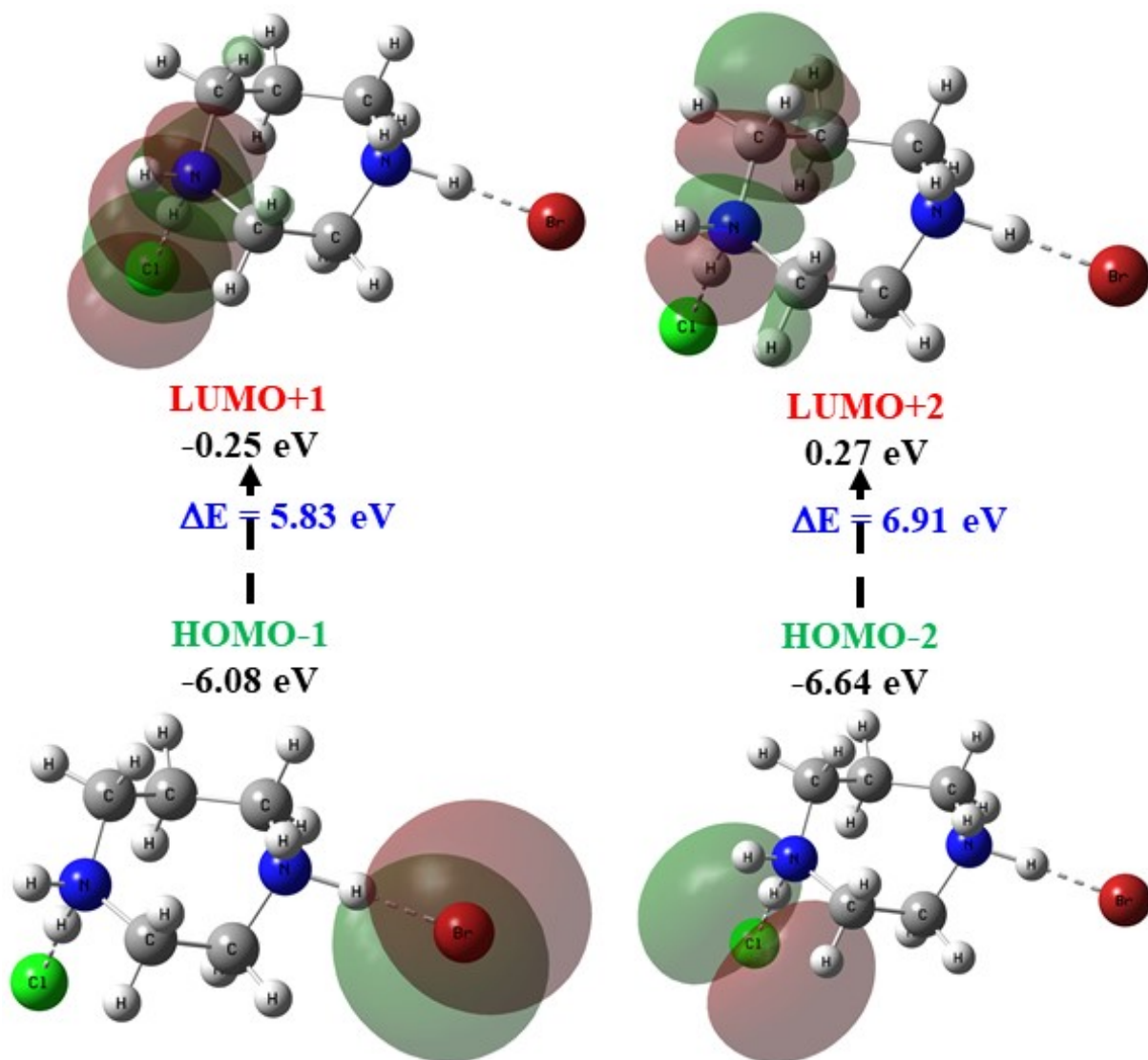


Figure S1. Frontier molecular orbitals of $(\text{C}_5\text{H}_{14}\text{N}_2)\text{BrCl}$: (a) HOMO-2, (b) HOMO-1, (c) HOMO, (d) LUMO, (e) LUMO+1, (f) LUMO+2.