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

Helicoidal Supramolecular Arrangement of (1R,2S)-Ephedrine within the AFI Structure: Towards a Transfer of Chirality to Mg Spatial Distribution

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Supporting Information

Inter-dimer angles, defined as the rotation angle around the c (channel) axis between the planes of the aromatic rings of consecutive dimers, were calculated as the average of the two torsion angles between C_m(dim1)-$C_{m'}$(dim1)-$C_{m'}$(dim2)-C_m(dim2) atoms of the two molecules composing the dimer, where C_m and $C_{m'}$ corresponds to the two *meta*-C atoms of EPH:

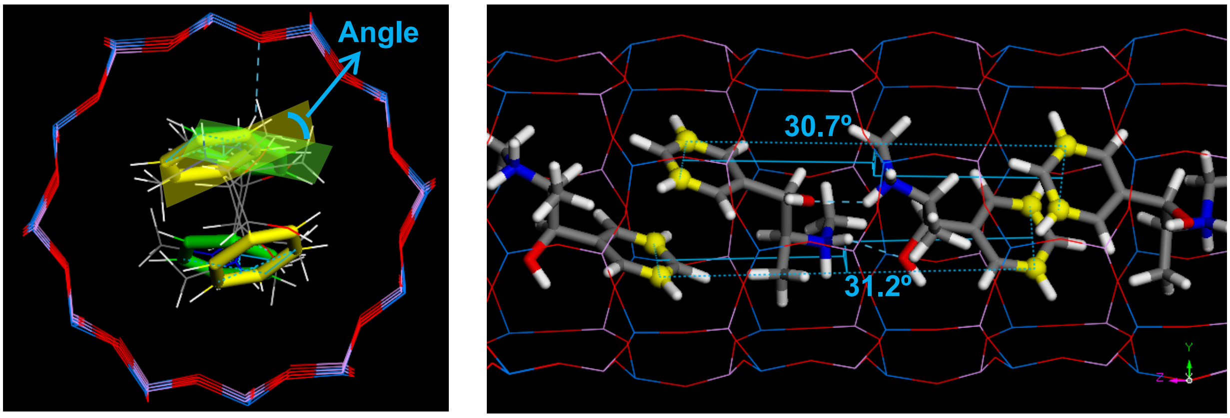

Figure S1. Definition of the inter-dimer angle as the angle between the planes of the aromatic rings of EPH molecules in consecutive dimers (left), calculated as the average between the two torsion angles between the C_m and $C_{m'}$ atoms of consecutive dimers.

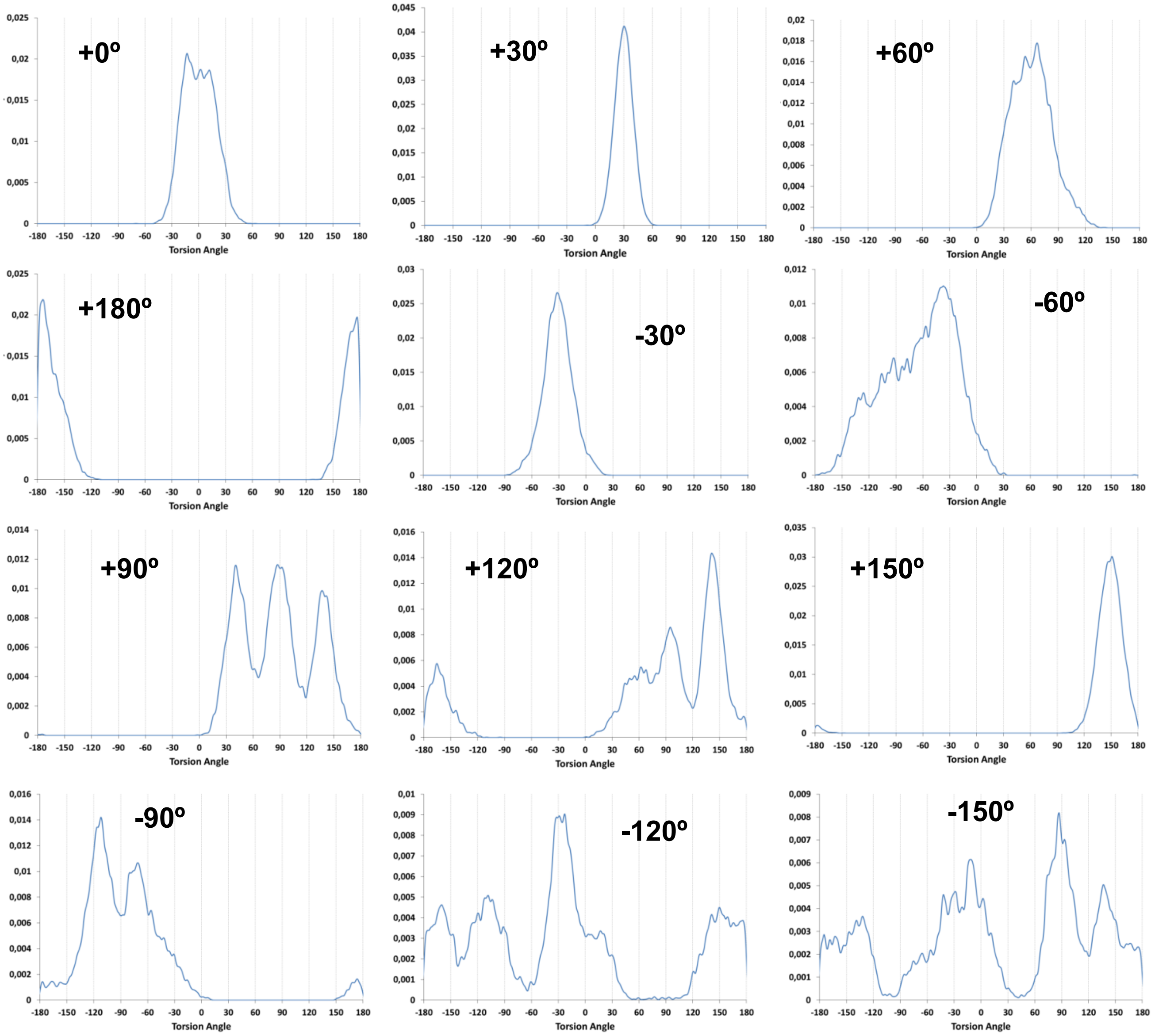

Figure S2. Inter-dimer angle distribution of 18AFI-24EPH systems with different initial angles during the MD simulations.

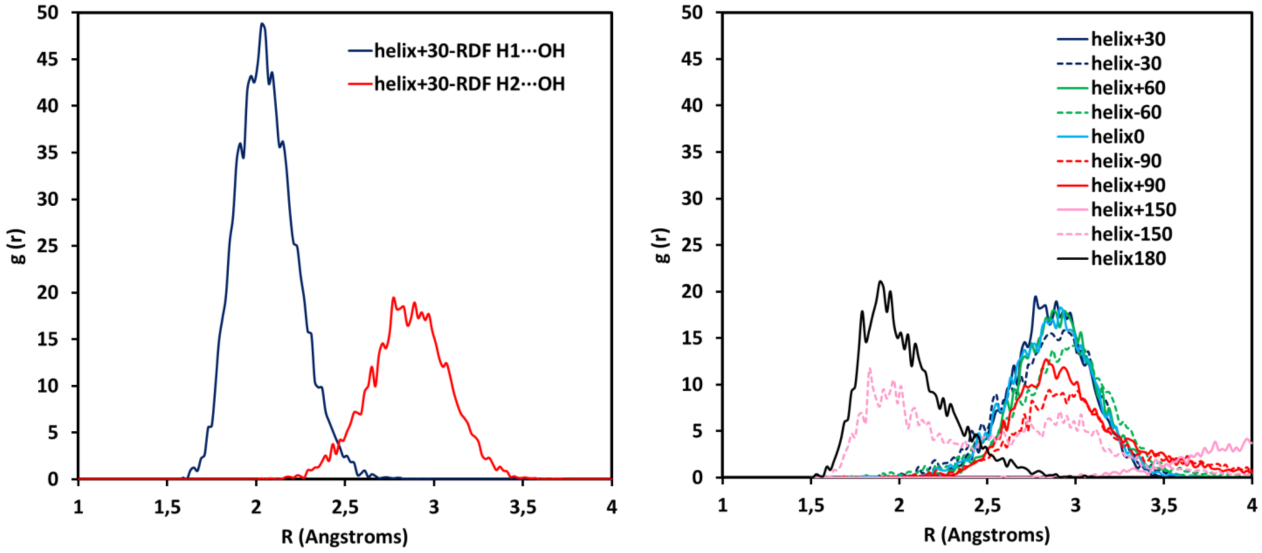

Figure S3. Left: Intermolecular H-bond formation as a function of H(N) atom for the helix+30 system: RDF (during the MD simulations) between O and H(1)-N (blue line) or H(2)N (red line) atoms. Right: Intermolecular H-bond formation with H(2)N atoms for the different systems: RDF (during the MD simulations) between O and H(2)-N atoms.

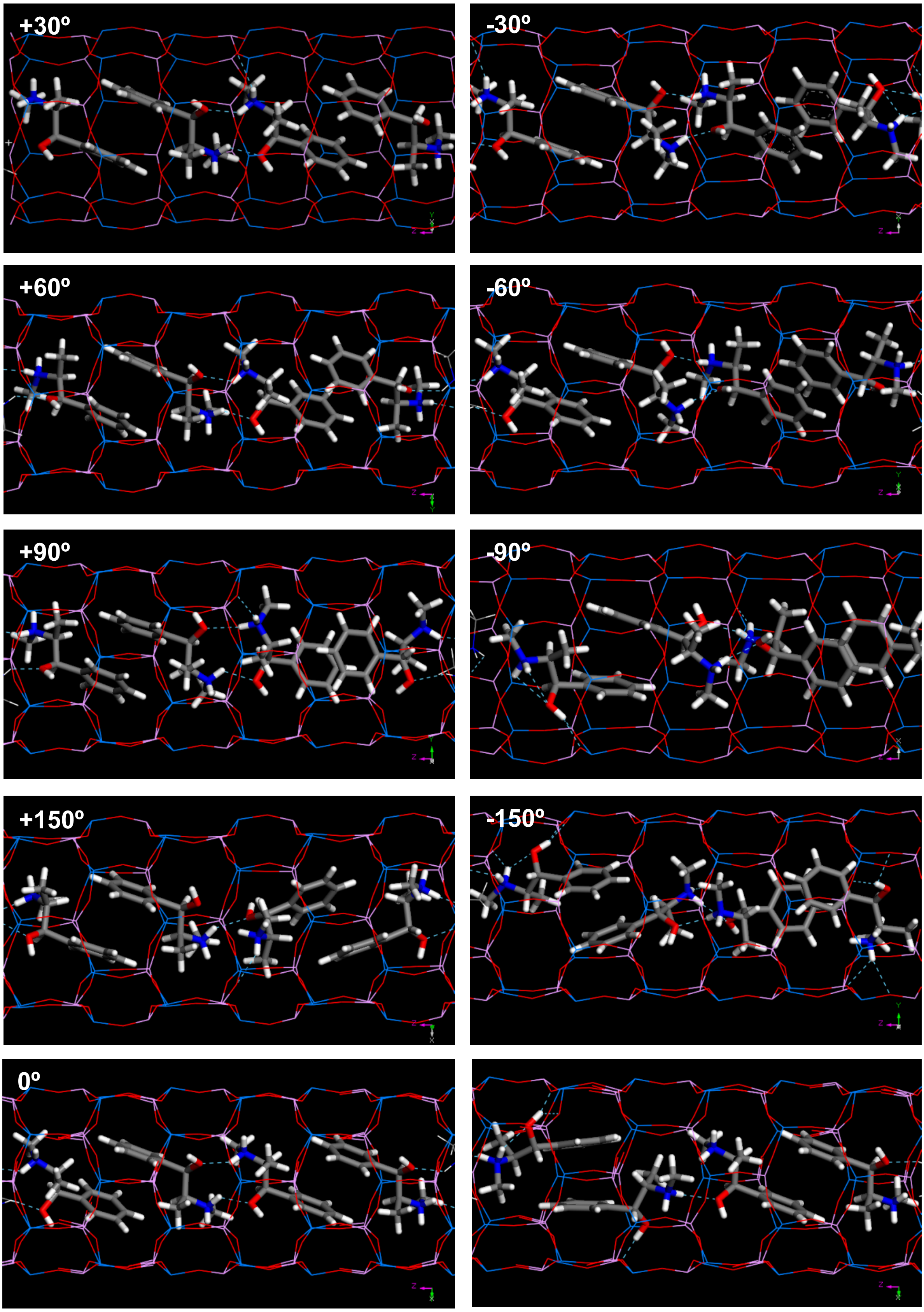

Figure S4. Arrangement of (1R,2S)-EPH dimers at different rotation angles in the undoped AFI systems (after MD+GO) (24EPH-18AFI model).

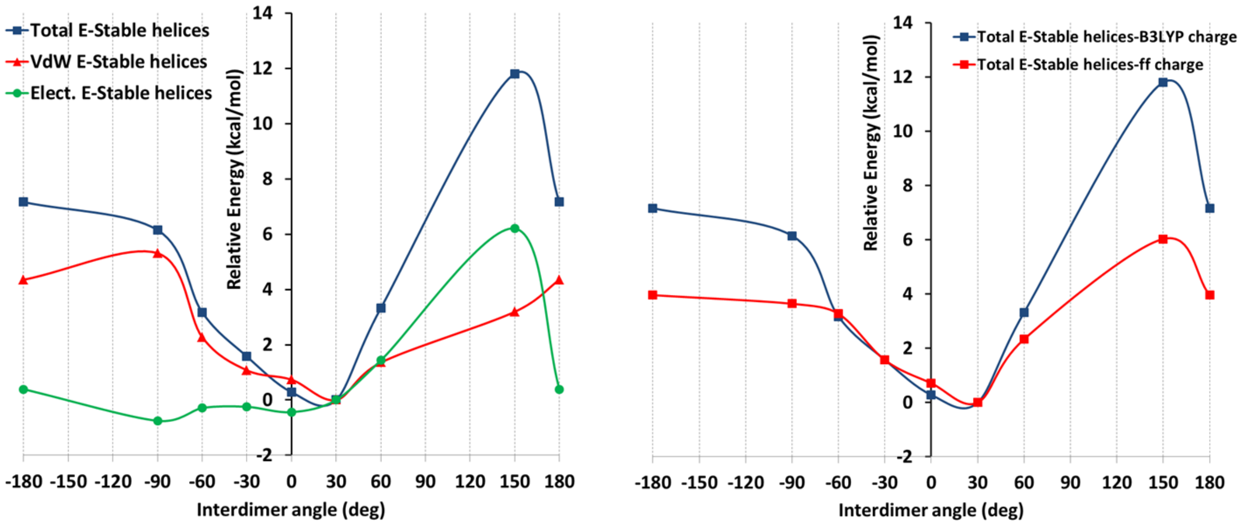

Figure S5. Left: interaction energy (in kcal/mol per u.c.) of the relaxed systems after MD and GO (model 18AFI-24EPH), decomposed in Van der Waals and electrostatic terms; right: interaction energy (in kcal/mol per u.c.) of the relaxed systems after MD and GO (model 18AFI-24EPH) as a function of the atomic charge distribution (blue: B3LYP charges: red: force-field-assigned charges).

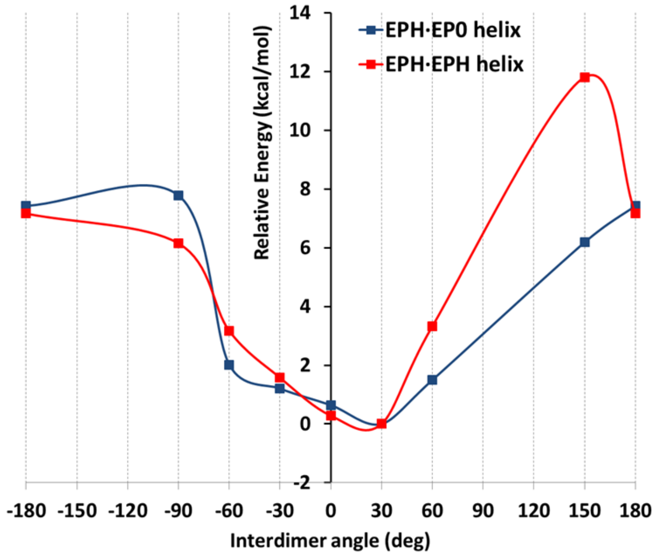

Figure S6. Interaction energy (in kcal/mol per u.c.) of the relaxed systems after MD and GO (model 18AFI-24EPH) as a function of the interdimer angle, for a system with all protonated EPH molecules (red line) and half protonated and half neutral molecules (blue line).

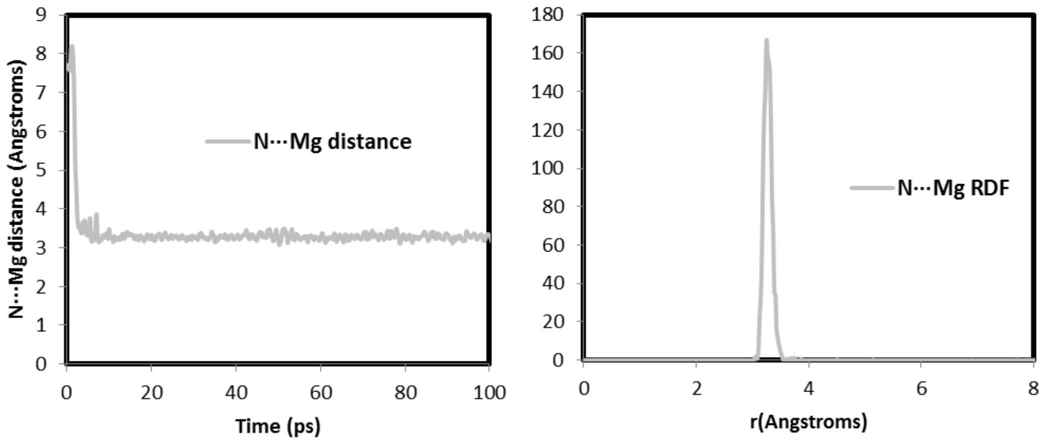

Figure S7. N···Mg distance as a function of the simulation time (left) and corresponding RDF (right) for a system with 1 Mg in a 1x1x3 AFI supercell with one protonated EPH loaded.

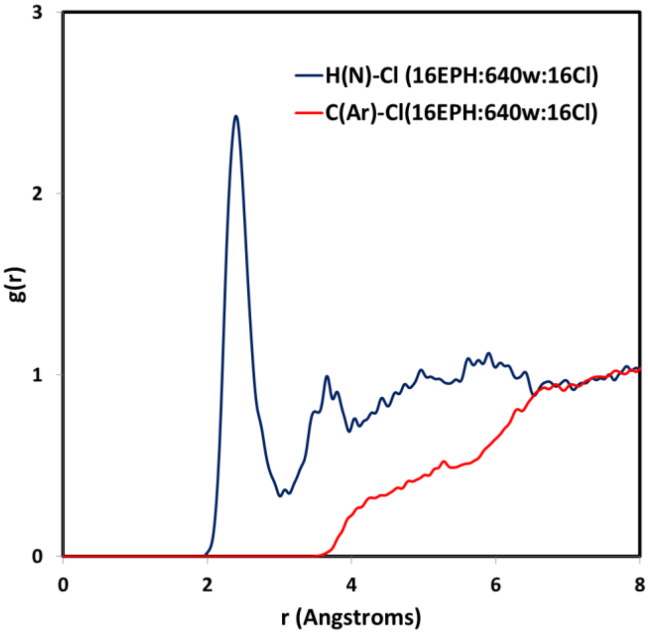

Figure S8. Radial Distribution Functions between H(N) atoms and Cl^- anions (blue line) and between aromatic C atoms and Cl^- anions (red line) during simulations in water (model 16EPH:640w:16Cl; see ref. 31 for details).