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ELECTRONIC SUPPORTING INFORMATION

Solvent effects on the properties of hyperbranched polythiophenes

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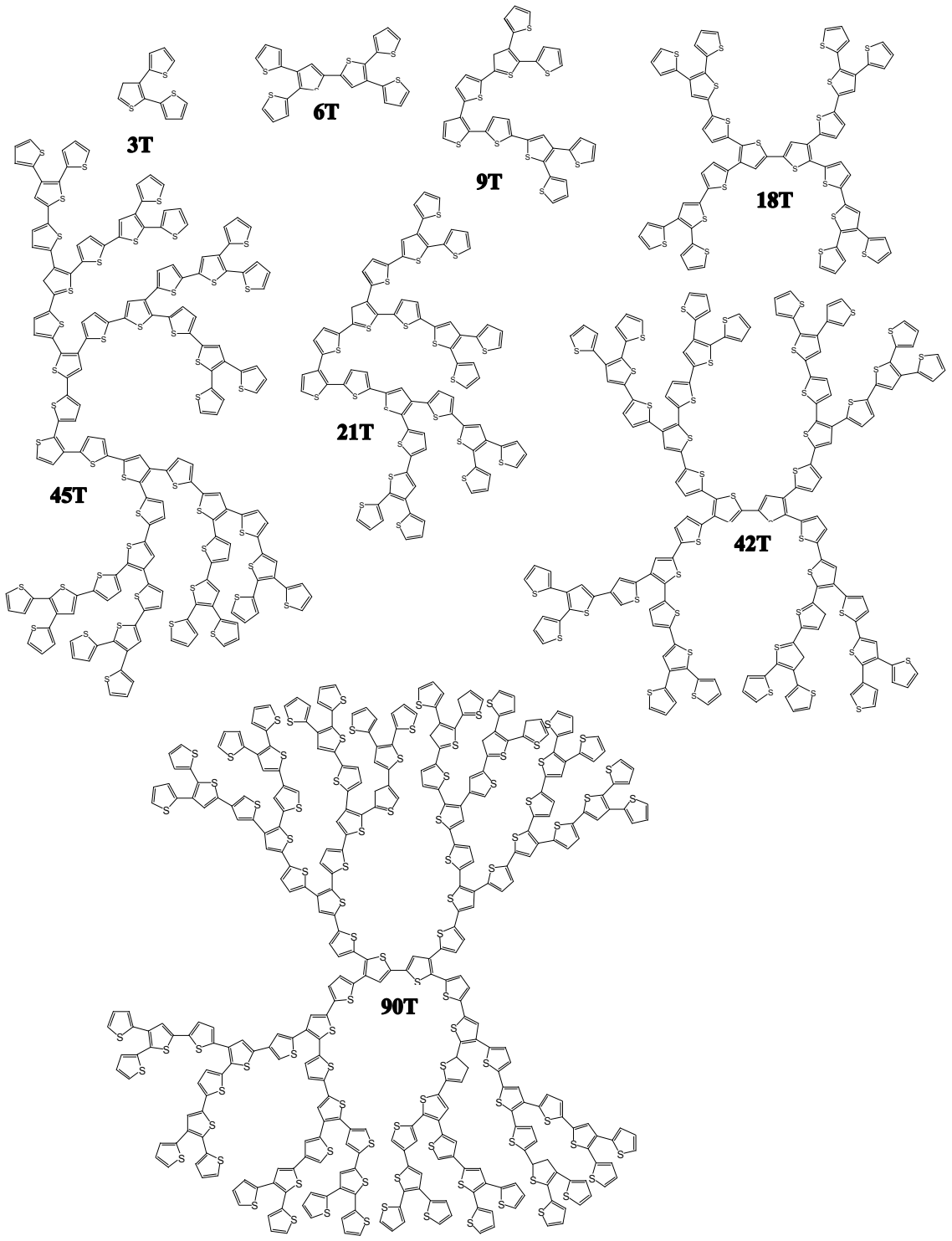

Figure S1. Chemical structure of dendrons and dendrimers studied in this work.

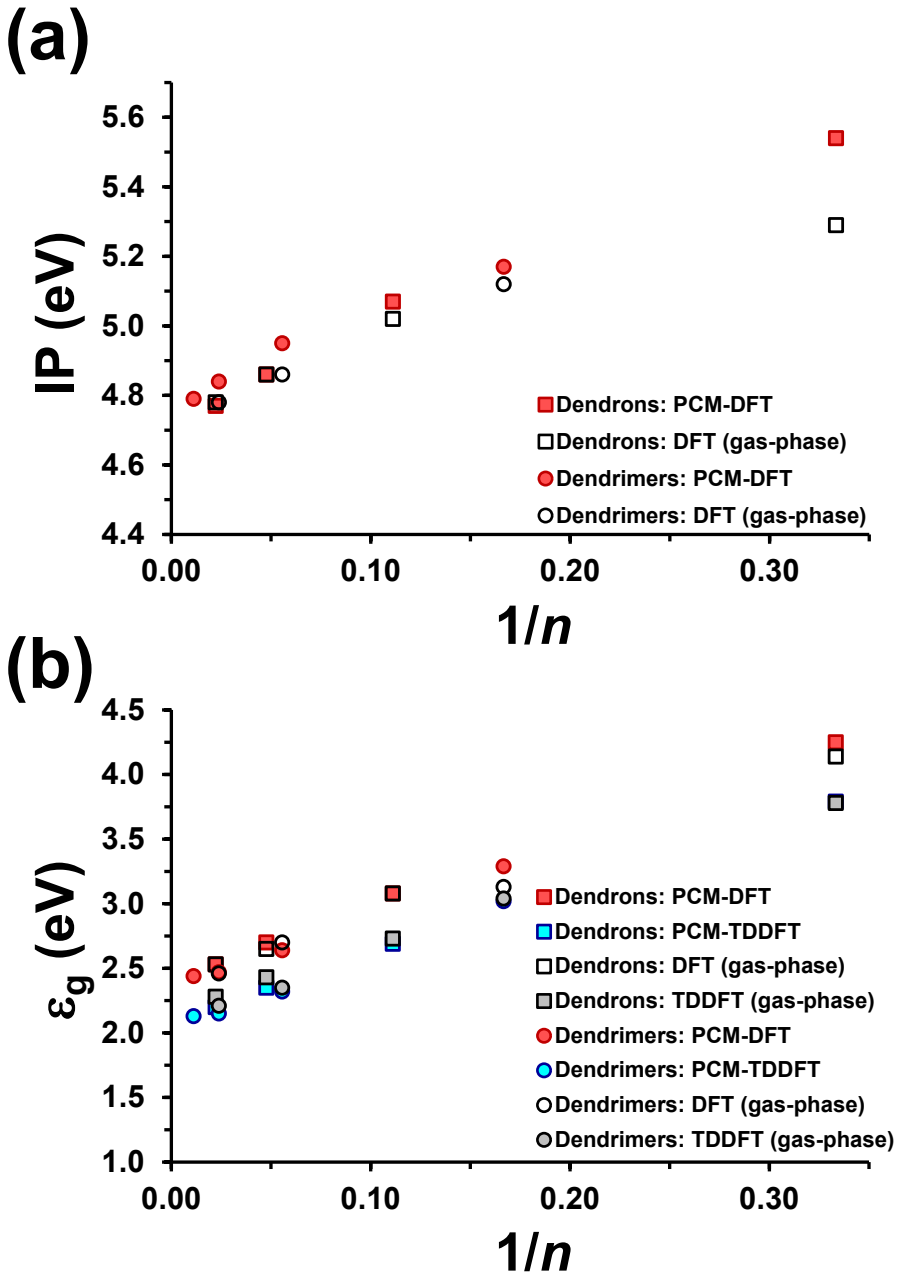

Figure S2. (a) Variation of the (a) IP and (b) ε_g against $1/n$, where n is the number of thiophene rings. Values derived from PCM-DFT and PCM-TD-DFT calculations in dichloromethane and from gas-phase calculations (taken from references 25 and 26).

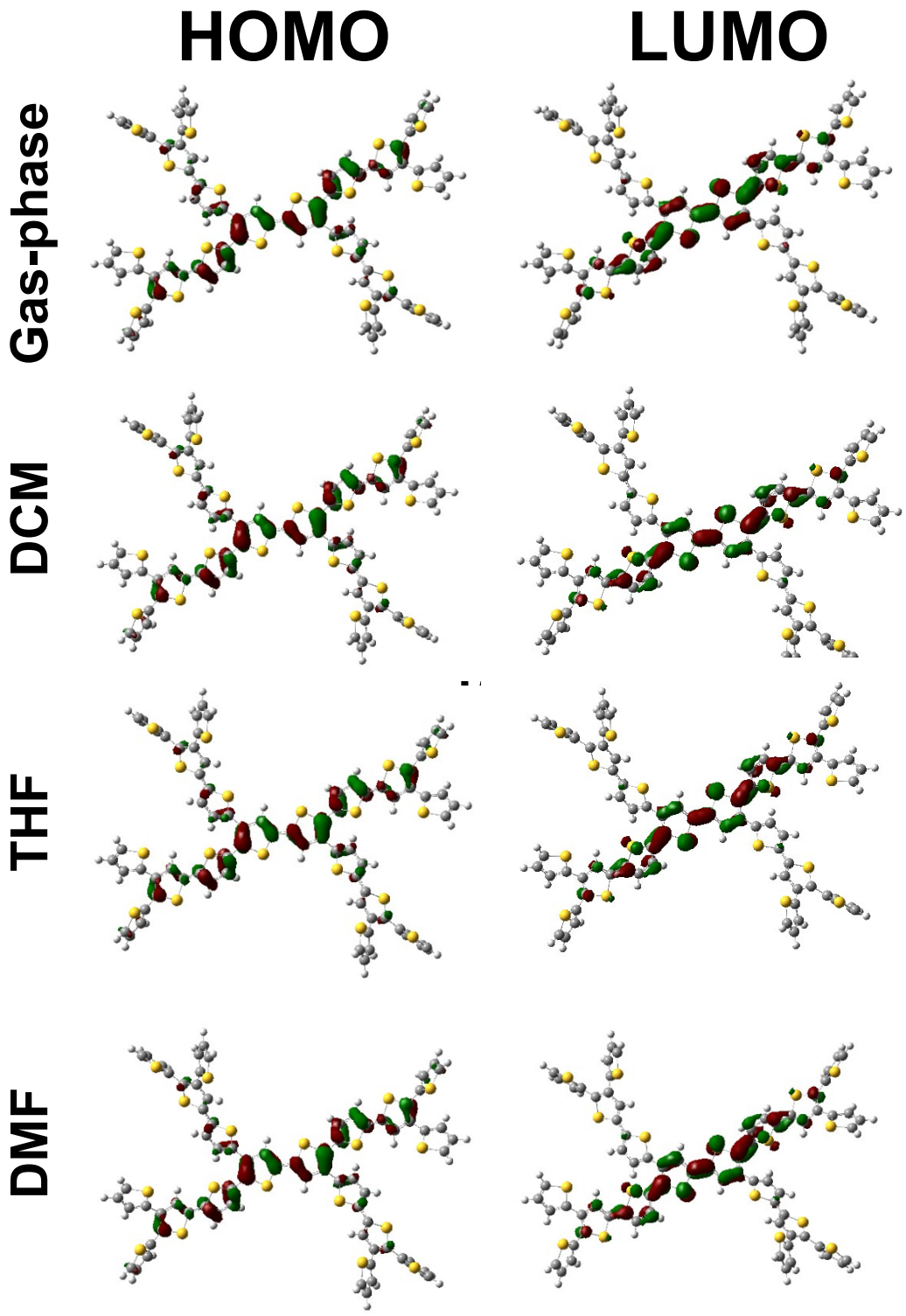

Figure S3. HOMO and LUMO frontier molecular orbitals 6T calculated in the gas-phase (B3LYP/6-31G(d)) and in DCM, THF and DMF solutions (PCM-B3LYP/6-31G(d)).

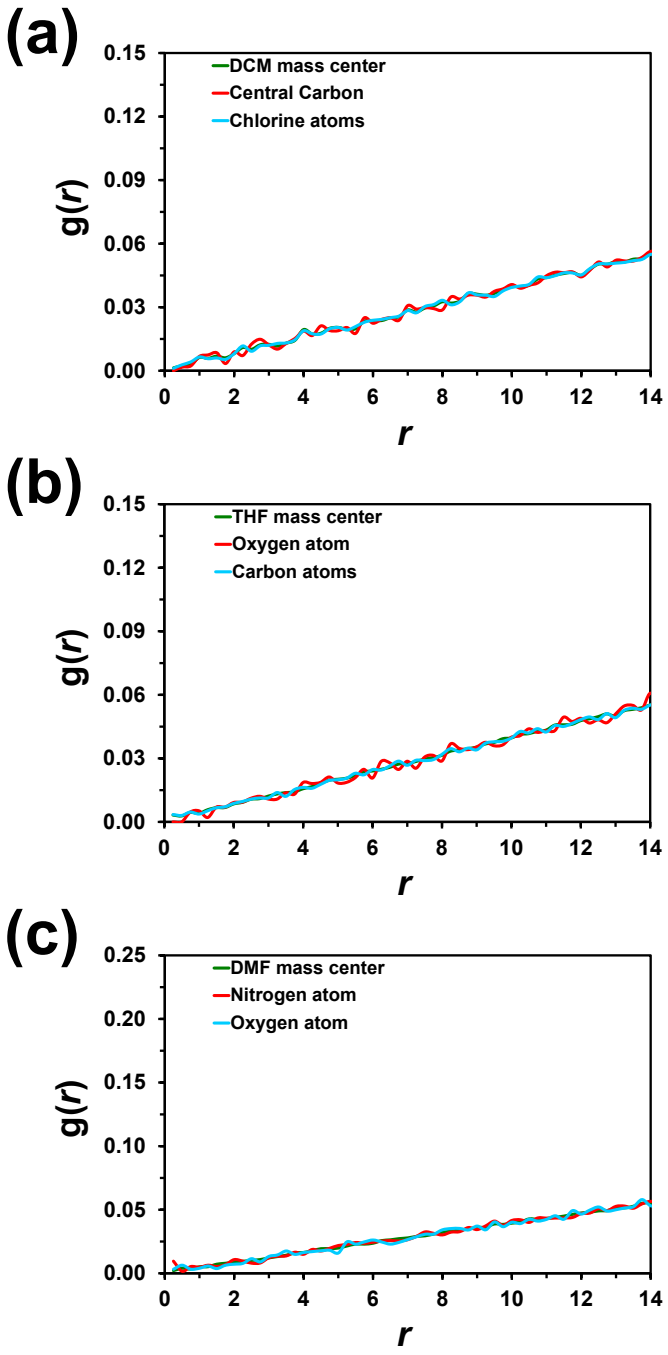

Figure S4. Distribution of solvent molecules as a function of the distance from the geometric center of the Th rings for 18T. The *g*(*r*) were calculated considering: (a) the center of masses, the chlorine atoms and the carbon atoms of the DCM molecules; (b) the center of masses, the oxygen atom and the carbon atoms of the THF molecules; and (c) the center of masses, the nitrogen atom and the oxygen atom of the DMF molecules.

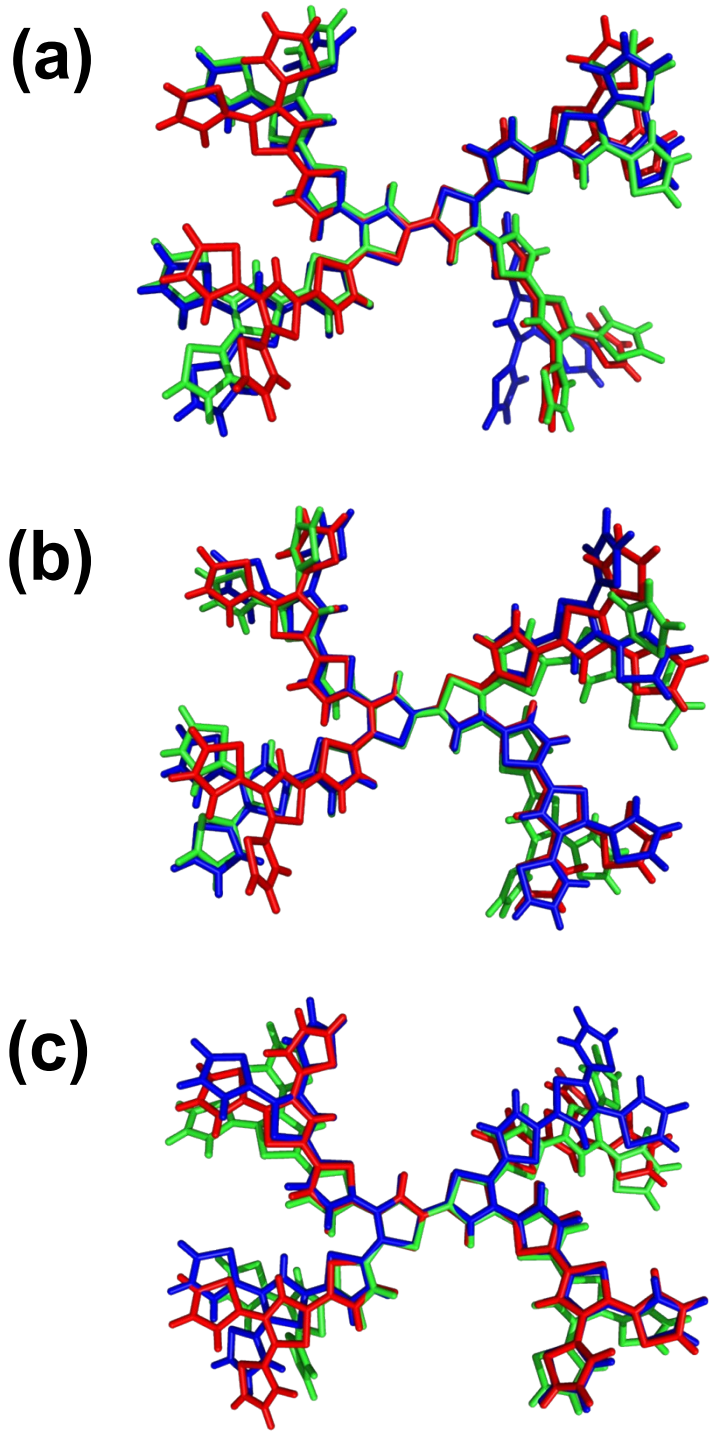

Figure S5. Superimposed structures of 18T extracted from snapshots at 5, 50 and 100 ns during MD trajectories in (a) DCM, (b) THF and (c) DMF.

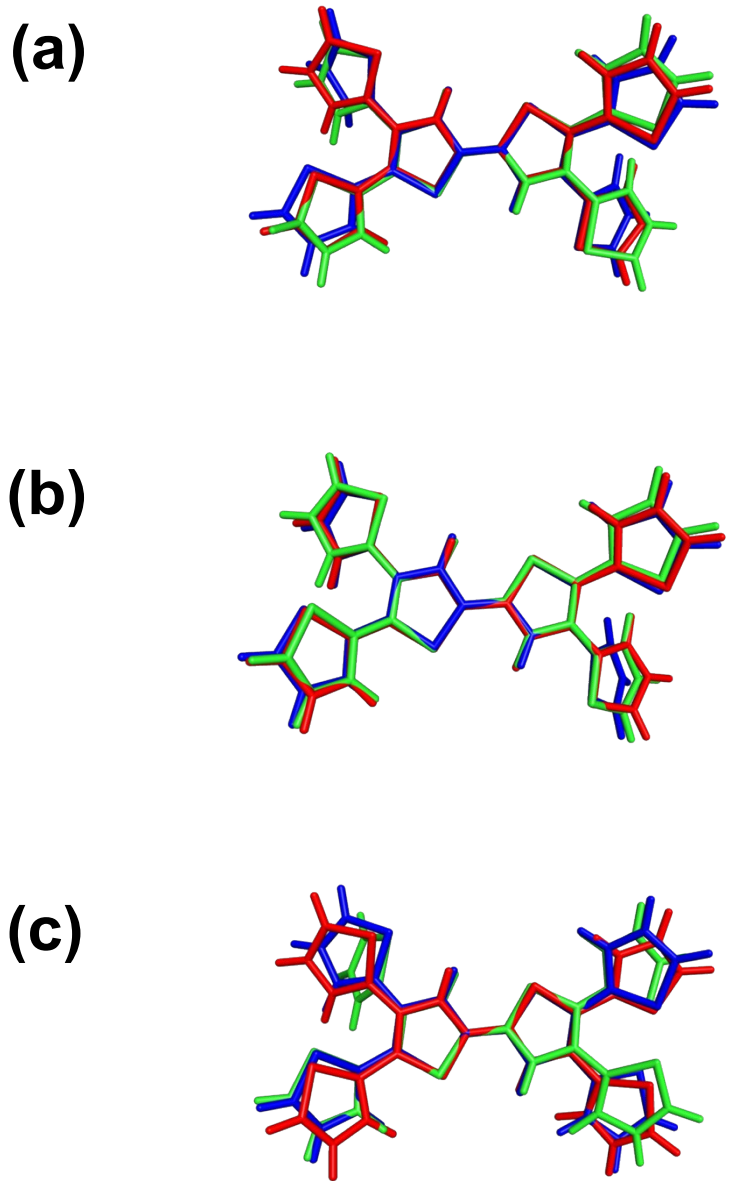

Figure S6. Superimposed structures of 6T extracted from snapshots at 5, 50 and 100 ns during MD trajectories in (a) DCM, (b) THF and (c) DMF.