

Supplementary materials

Sm/Co Magnetic Materials: A Recycling Strategy Using Modifiable Hydrophobic Deep Eutectic Solvents Based on Trioctylphosphine Oxide

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Table S1. Materials

Compound	Supplier	CAS	Purity, wt% *
Trioctylphosphine oxide	Acros	78-50-2	98%
Thymol	Acros	89-83-8	99%
Phenol	Chimmed	108-95-2	99%
p-tert-Butylphenol	Chimmed	98-54-4	99%
HNO ₃	Chimmed	7697-37-2	—
Sm(NO ₃) ₃ ·6H ₂ O	Chimmed	13759-83-6	99%
Co(NO ₃) ₂ ·6H ₂ O	Chimmed	10026-22-9	99%
NaNO ₃	Chimmed	7631-99-4	99%

*Declared by suppliers.

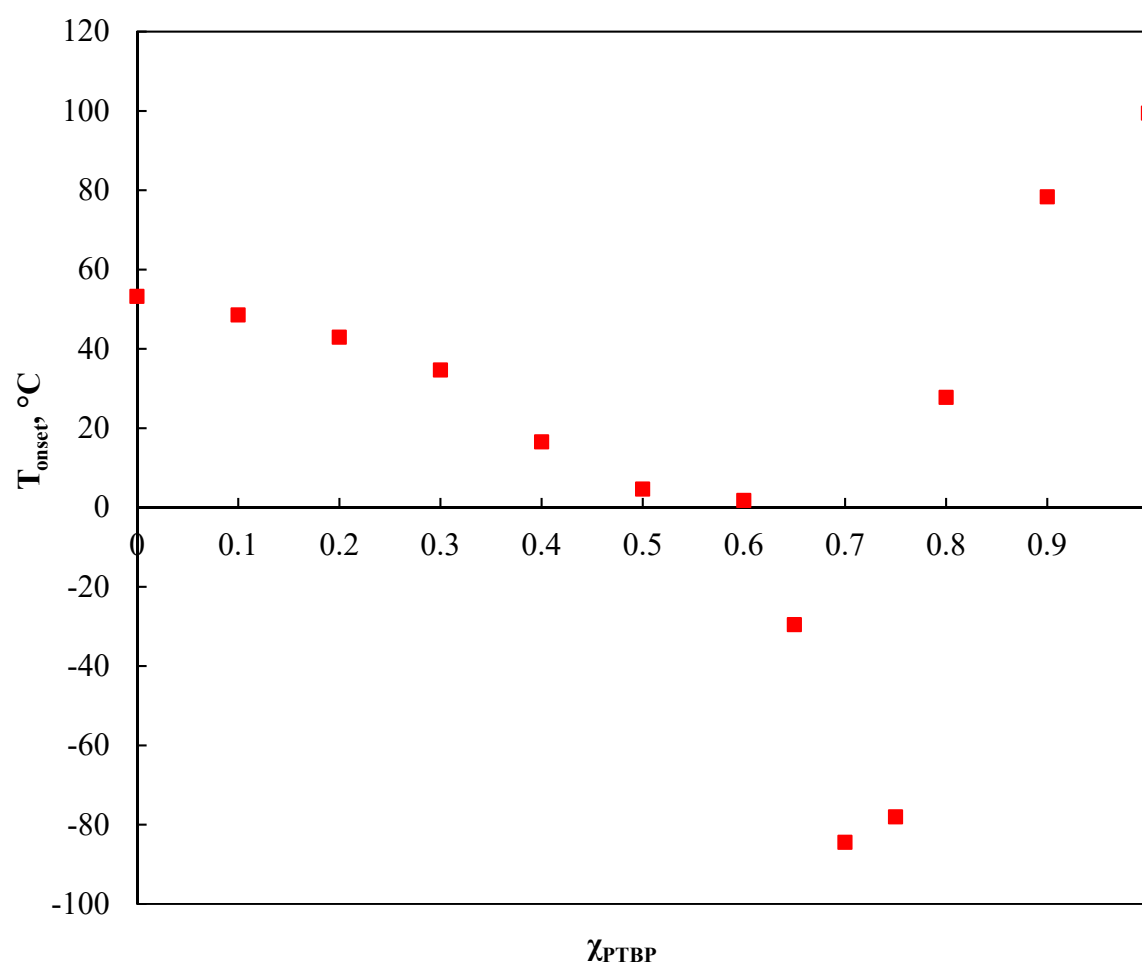


Figure S1. Phase diagram for PTBP:TOPO mixture, constructed from DSC results.

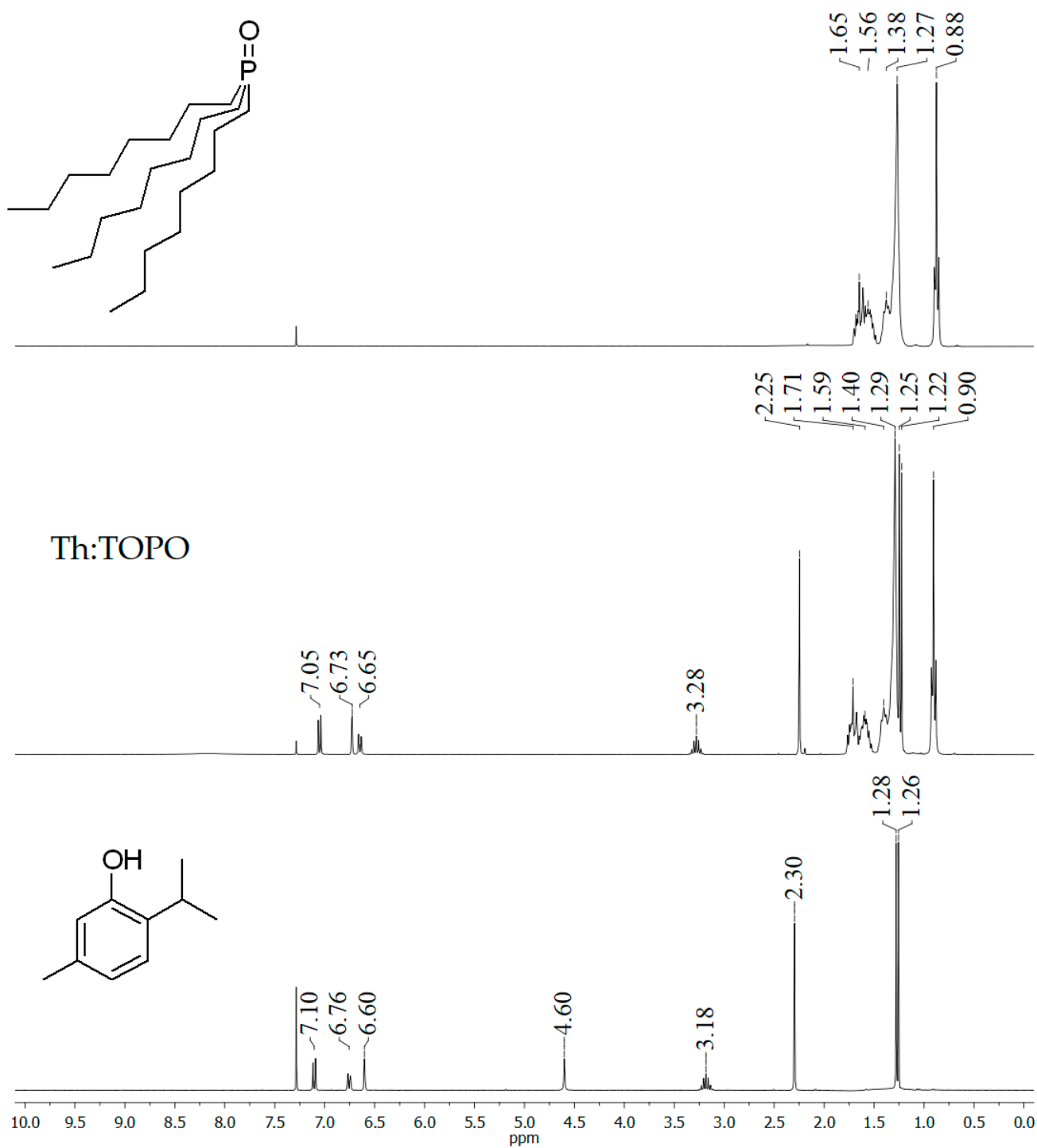


Figure S3. Proton NMR of Th:TOPO HDES.

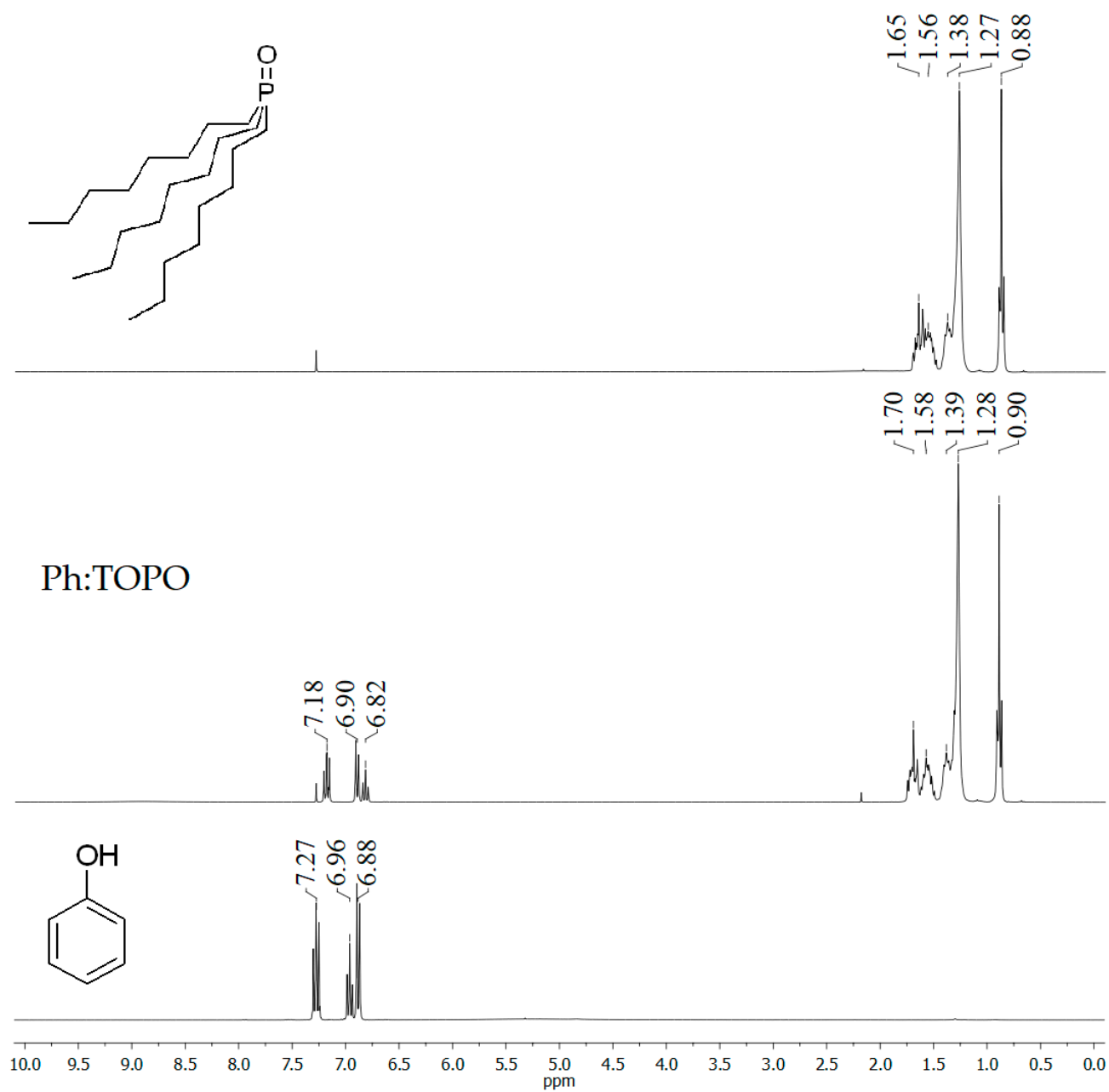


Figure S4. Proton NMR of Ph:TOPO HDES.

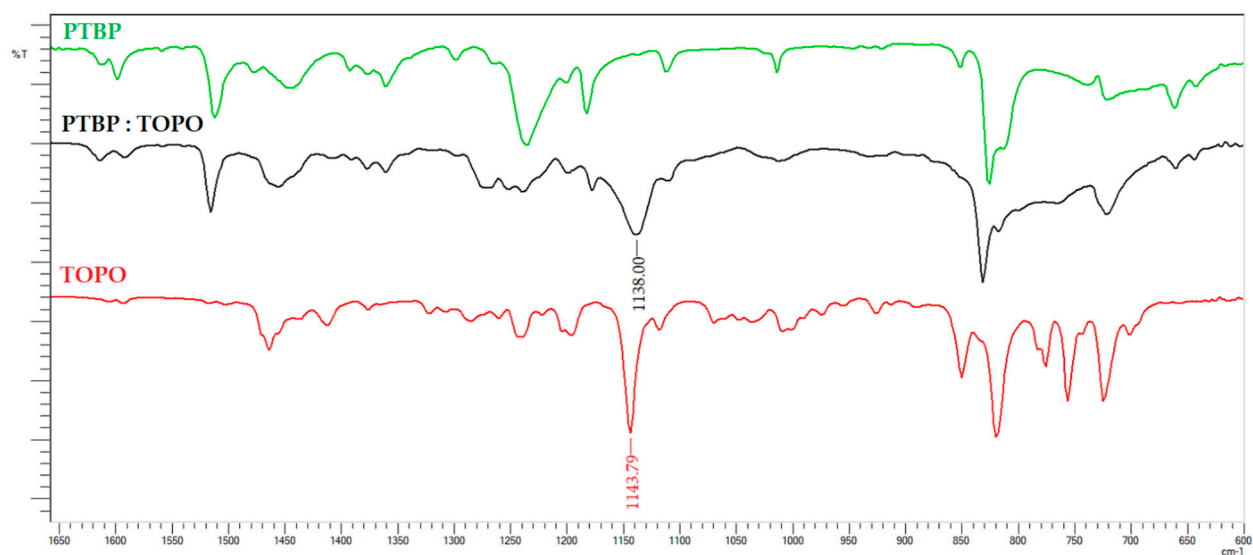


Figure S5. FTIR spectra of PTBP:TOPO HDES.

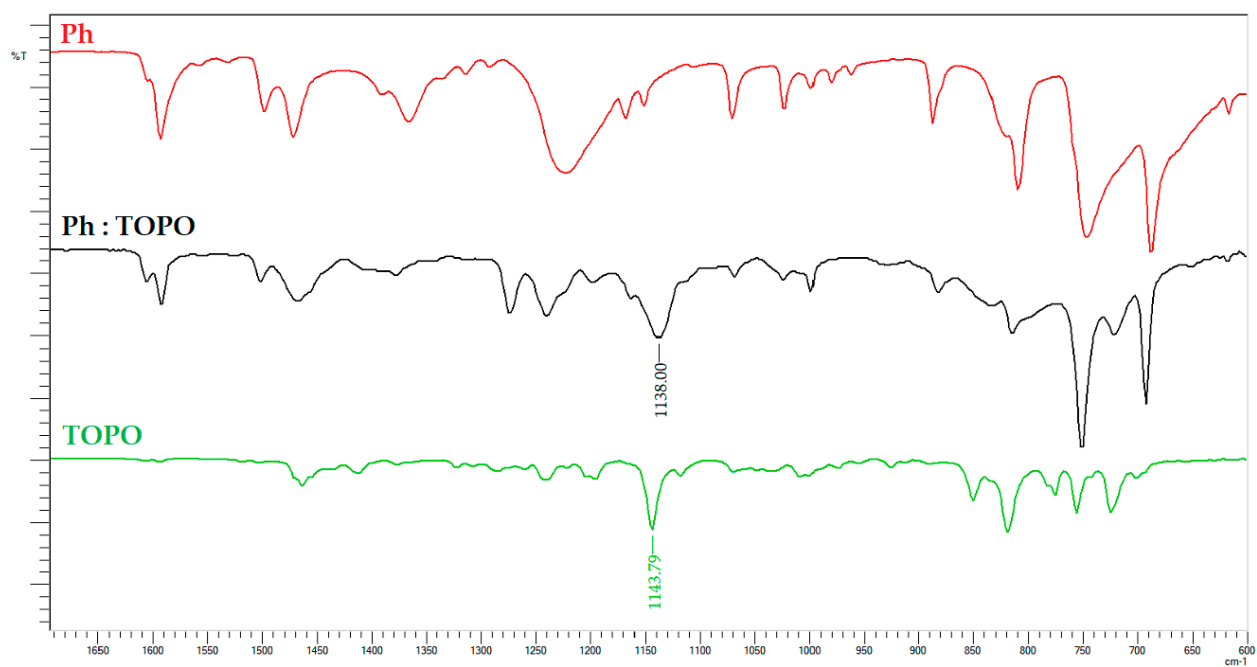


Figure S6. FTIR spectra of Ph:TOPO HDES.

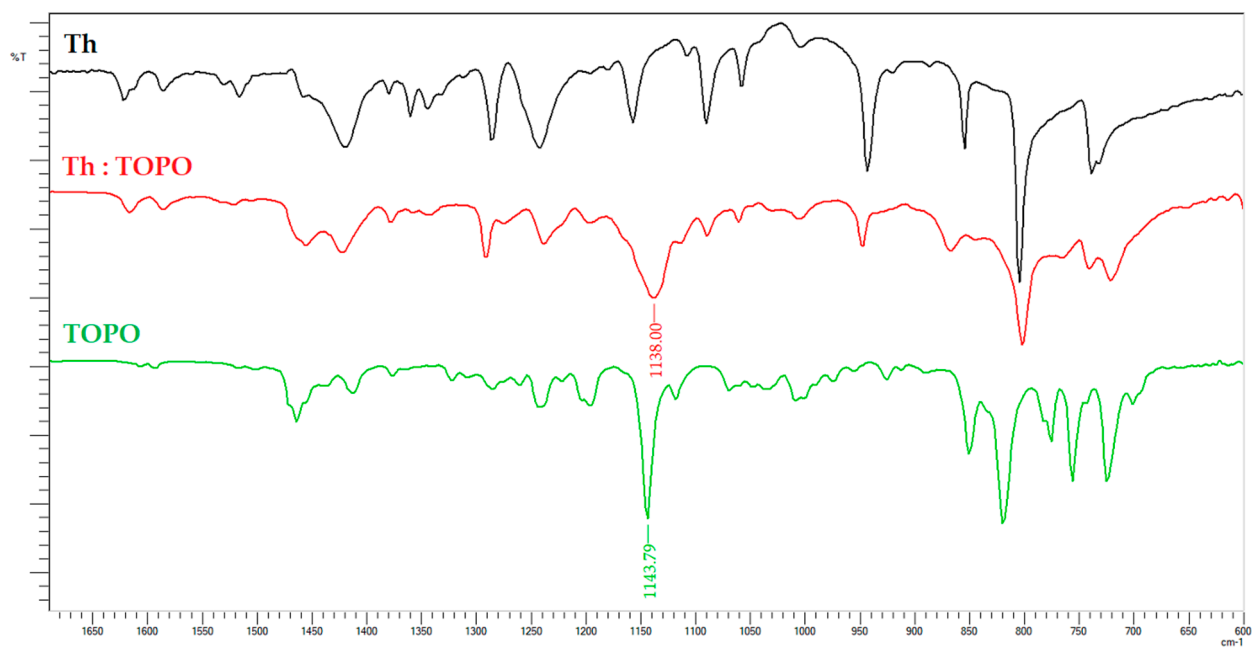


Figure S7. FTIR spectra of Th:TOPO HDES.

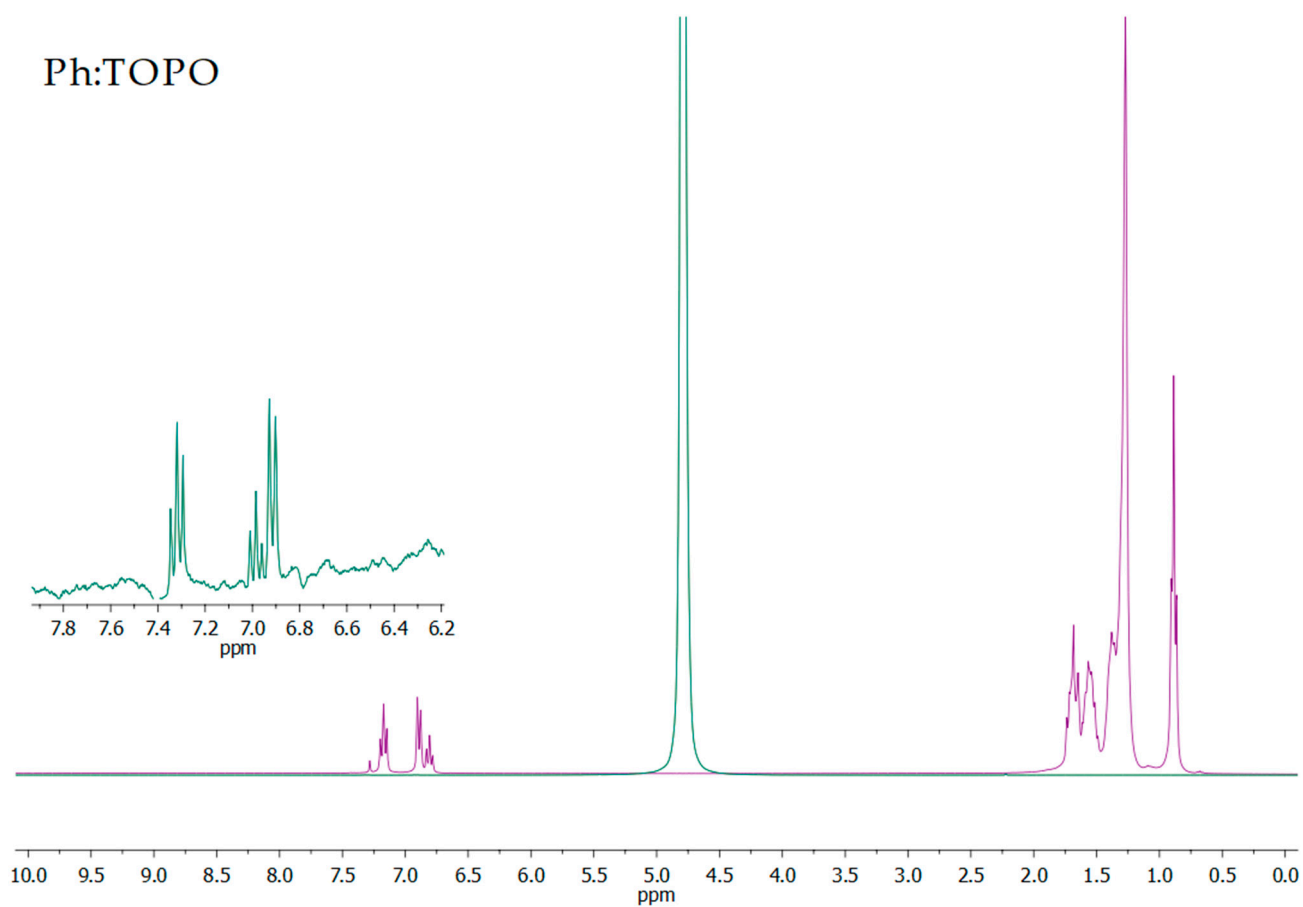


Figure S8. ¹H NMR spectra of the aqueous (green line) and HDES Ph:TOPO phases (purple line) after stirring.

PTBP:TOPO

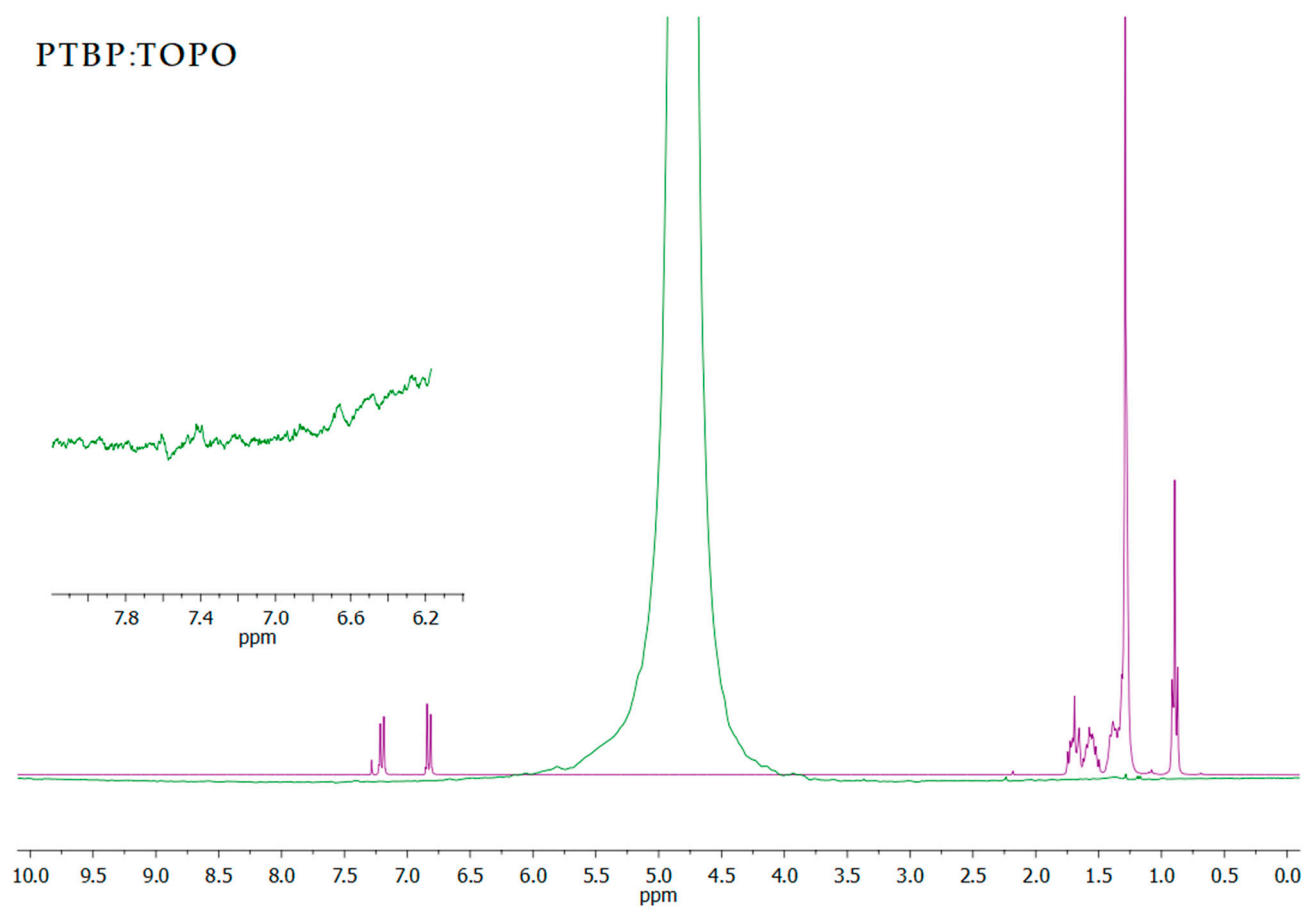


Figure S9. ^1H NMR spectra of the aqueous (green line) and HDES PTBP:TOPO phases (purple line) after stirring.

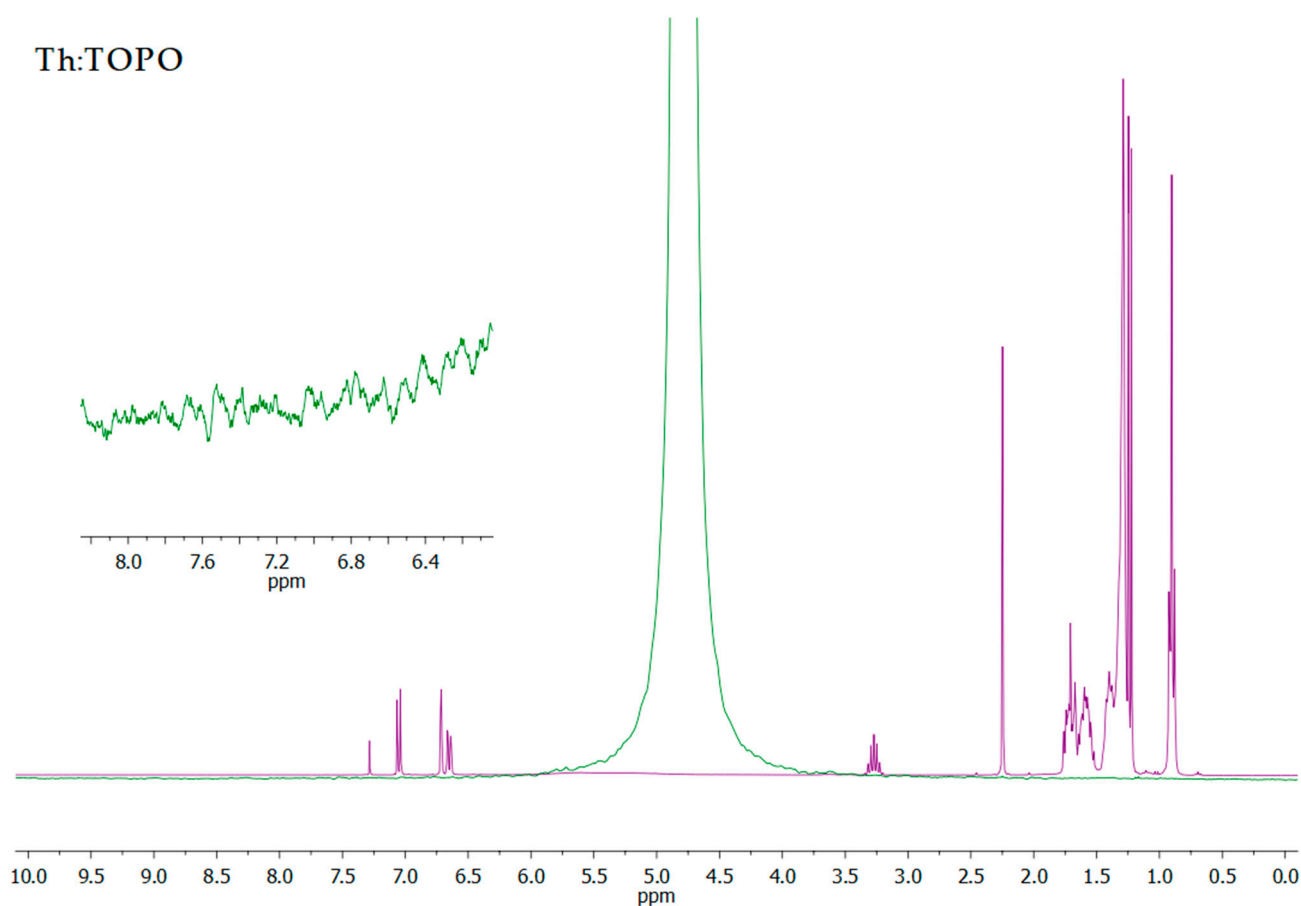


Figure S10. ^1H NMR spectra of the aqueous (green line) and HDES Th:TOPO phases (purple line) after stirring.

Computational study

Theoretical calculations: optimization of all molecular geometries, NBO (natural bond orbital) charges, supramolecular complexes energies were performed using Gaussian16 [1] software package at PBE-D3(BJ)/def2-TZVP level of theory. PBE [2] functional and Weigend def2-TZVP [3] basis set has recommended itself as a highly accurate method for modelling small organic molecules [4, 5]. Grimme's D3 dispersion correction with Becke–Johnson damping has been used to better estimation of non-covalent interactions [6]. BSSE correction energies computed using the counterpoise scheme [7]. Tight optimization criteria and ultrafine grids were used in each calculation.

References

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