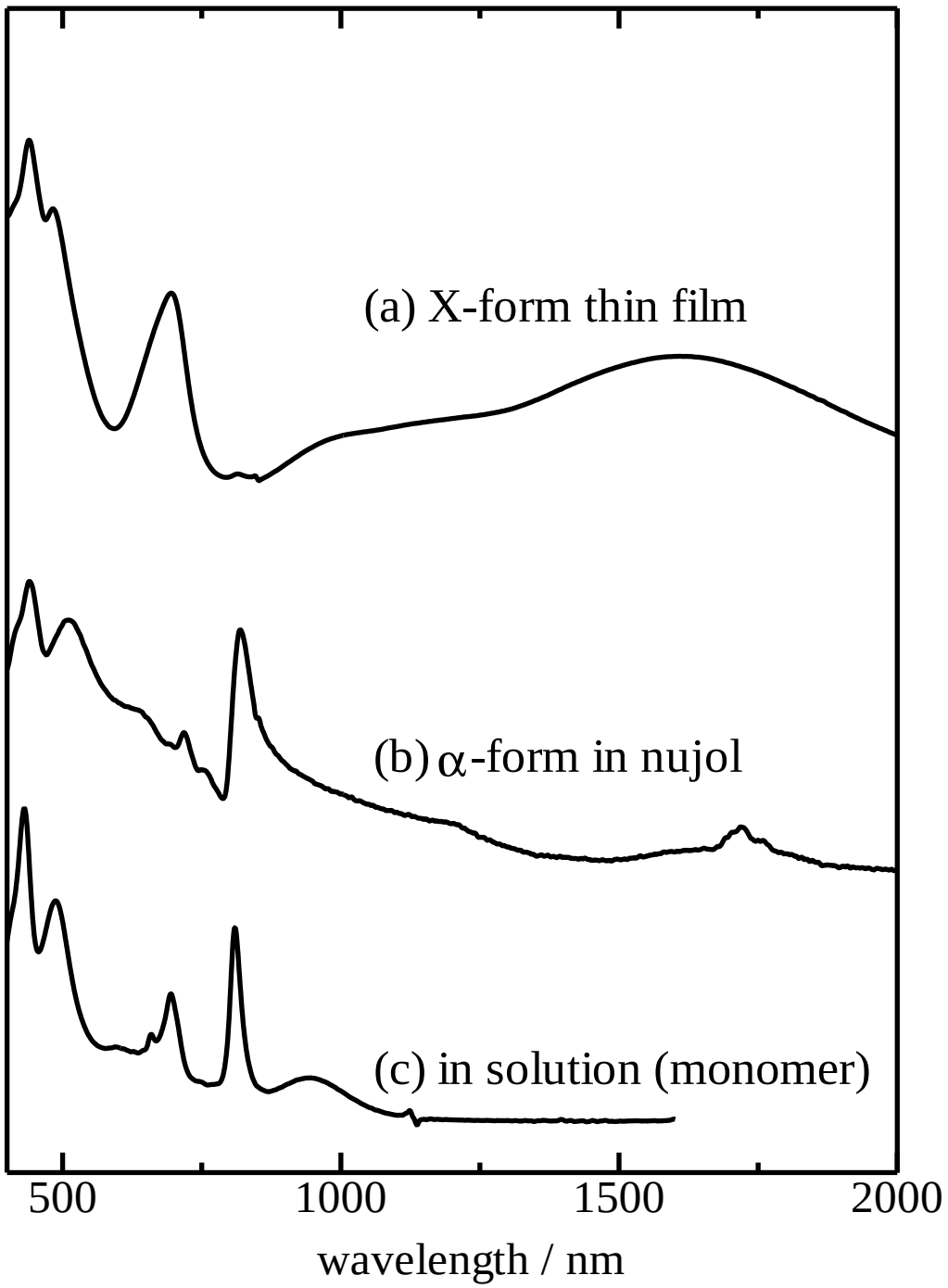
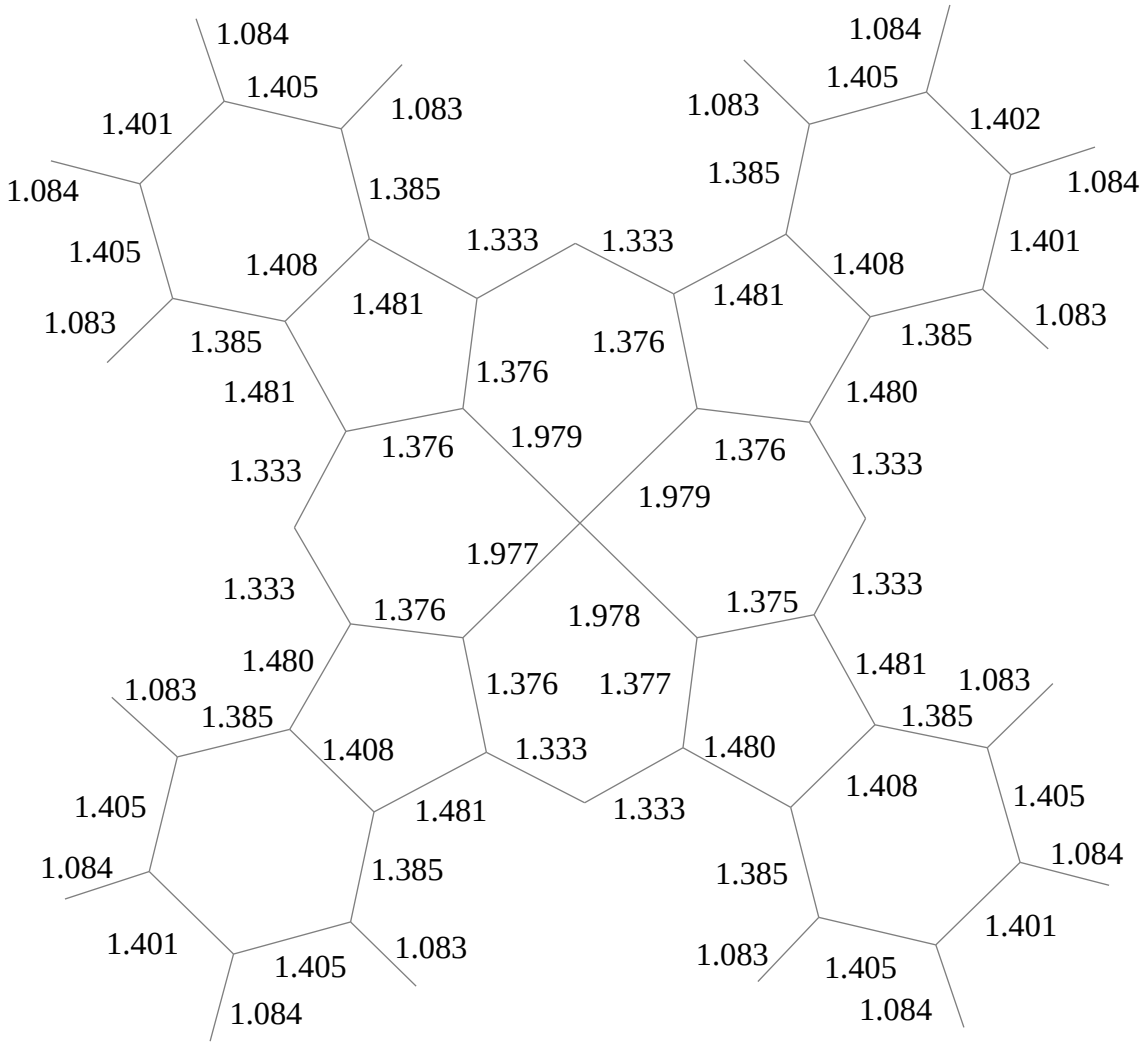
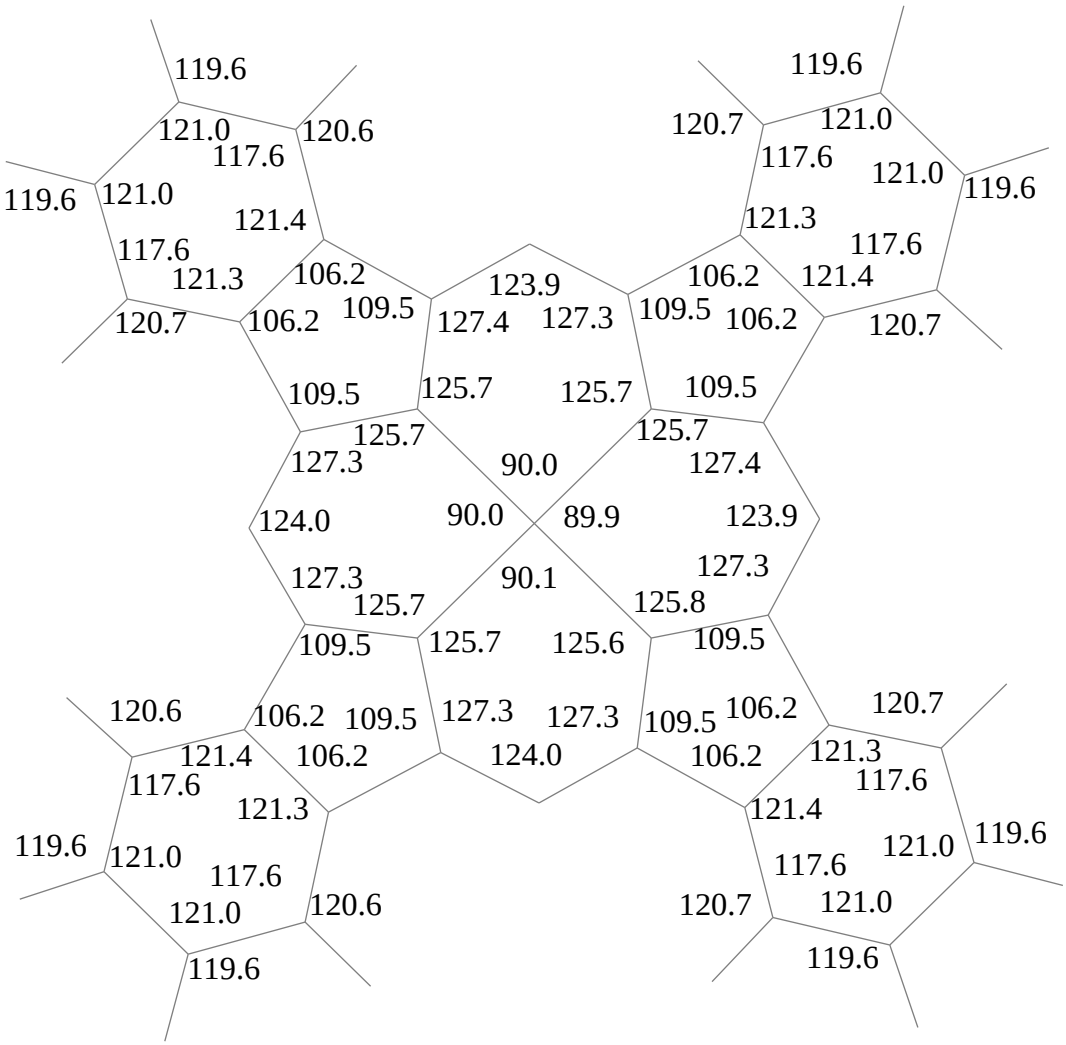


(Electronic Supplementary Information) Figure 1. Absorption spectra of LiPc for (a) the X-form in the thin film, (b) the α-form in nujol, and (c) the free monomer in o-dichlorobenzene solution. All polymorphs show the same spectrum in solution.



(Electronic Supplementary Information) Figure 2. Optimized geometry of LiPc. Bond length in angstrom.



(Electronic Supplementary Information) Figure 3. Optimized geometry of LiPc. Bond angle in degree.

(Electronic Supplementary Information) Table 1. Total energies of α- and β-type dimers obtained by the DFT method.

		α-type	β-type
ΔE^a / kcal mol^{-1}	singlet	–0.7	–3.1
	triplet	–6.5	–8.5

[a]The stabilization energy of dimers relative to two LiPc molecules.