

Electronic Supplementary Material

Effects of solvents and temperature on spherulites of self-assembled phloroglucinol tristearate

Yawen Yao¹, Sabine Rosenfeldt², Kai Zhang(✉)¹

¹ Wood Technology and Wood Chemistry, Georg-August-University of Goettingen, 37077 Göttingen, Germany

² Department of Chemistry and Bavarian Polymer Institute, University of Bayreuth, 95447 Bayreuth, Germany

E-mail: kai.zhang@uni-goettingen.de.

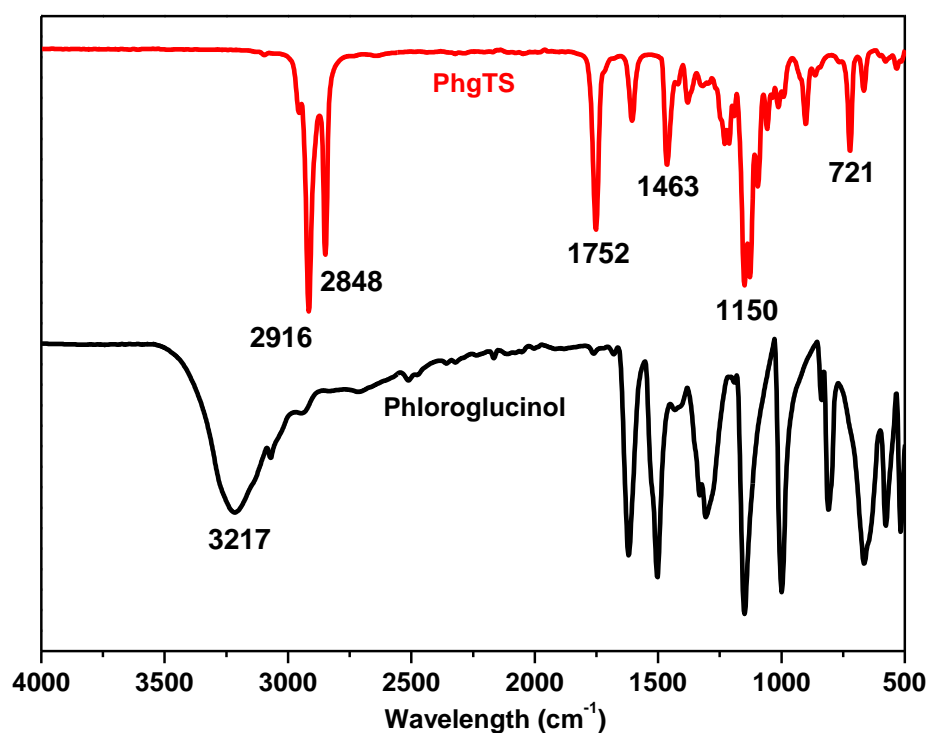


Figure S1. FT-IR spectra (4000-500 cm⁻¹) of phloroglucinol and PhgTS

FT-IR spectra show characteristic peaks of phloroglucinol and PhgTS (Figure S1). In the spectrum of phloroglucinol, the peaks near 3217 cm^{-1} represent OH groups, while these peaks disappeared in the spectrum of PhgTS. New bands appear at 2916 and 2848 cm^{-1} , which are attributed to the asymmetric and symmetric stretching vibrations of methylene groups, respectively. Another new signal at 1752 cm^{-1} is ascribed to the stretching vibrations of C=O groups and the new band at 1463 cm^{-1} is derived from the deformation vibrations of C-H groups of long aliphatic chains. In addition, new bands at 1150 and 721 cm^{-1} are ascribed to stretching and rocking vibrations of C-C groups of long aliphatic chains, respectively.

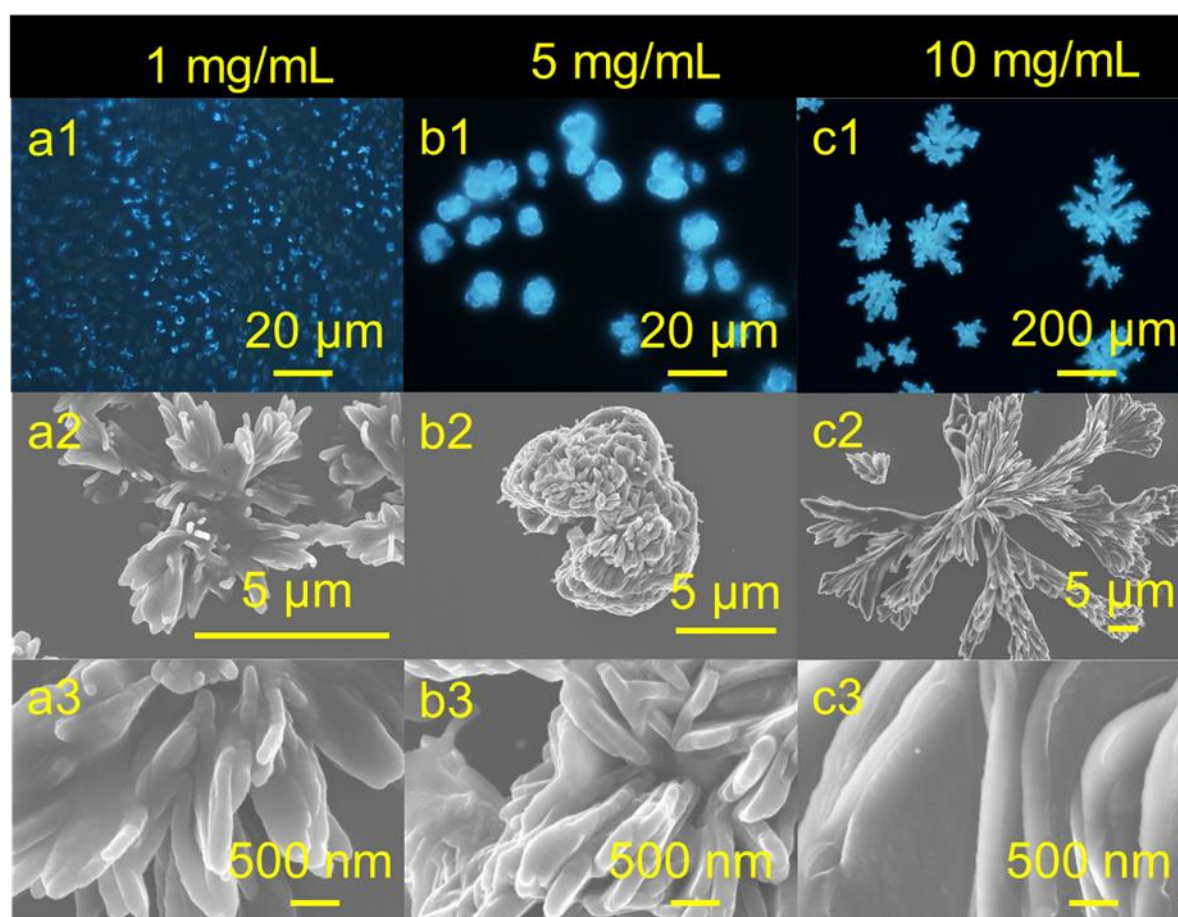


Figure S2. Morphologies of PhgTS crystals induced by 1-butanol with different concentrations. (a1-c1) Polarized optical microscope images of PhgTS crystals with the

concentration of 1, 5 and 10 mg/mL, respectively. (a2-c2) and (a3-c3) SEM images of PhgTS crystals in distinct magnifications.

When the concentration is 1 mg/mL, petal-like sheets can be observed. However, with the increasing of concentration to 5 mg/mL, sheet structures grow together to form nonuniform round aggregates. With the concentration of 10 mg/mL, clear cupressaceae leaves-like structures were obtained. The SEM image of the PhgTS self-assembled structure derived from 1-butanol solution confirms the formation of a branch-like structure (Figure S2).

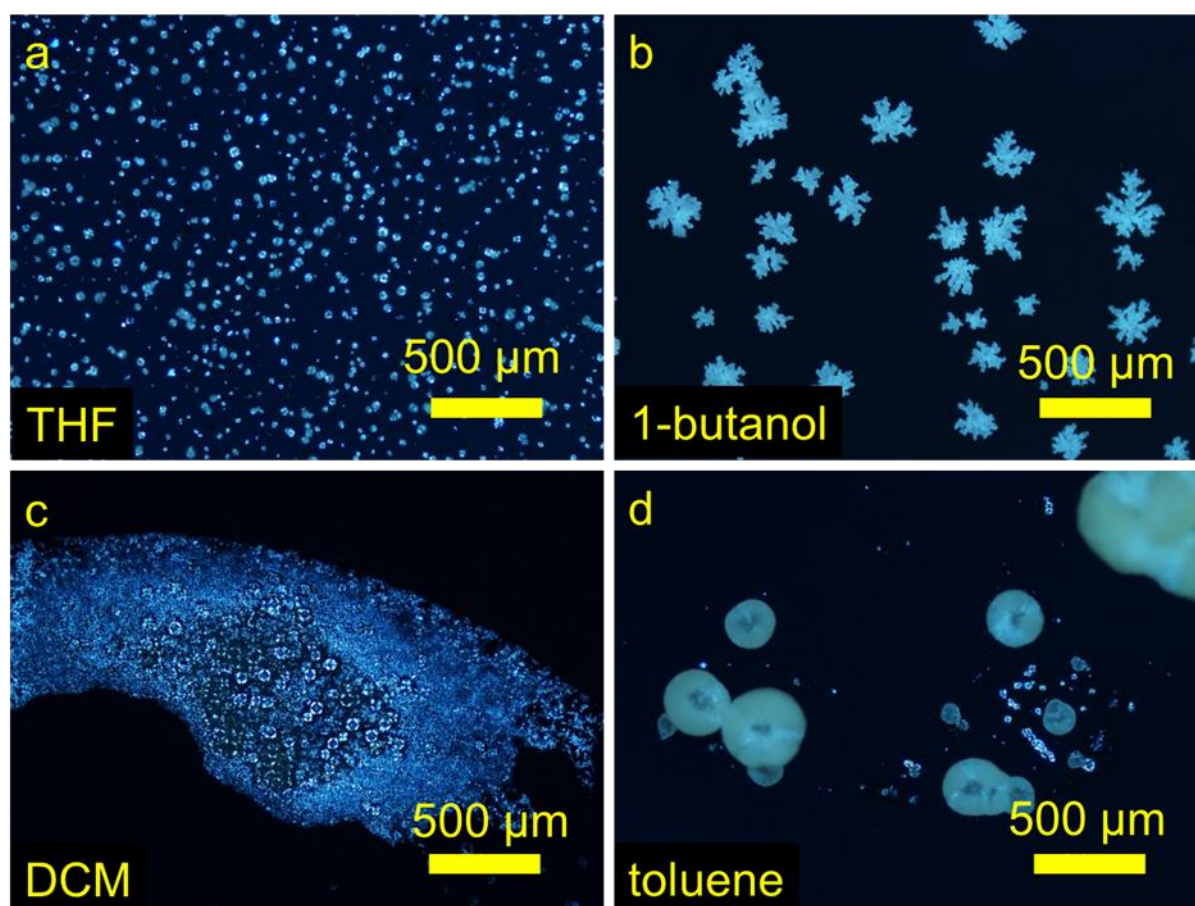


Figure S3. (a-d) Low magnification polarized optical microscope images of PhgTS crystals from its solution in THF, 1-butanol, DCM and toluene with the concentration of 10 mg/ml, respectively.

For further understanding of the crystals formed from these 4 types of solvents, low magnification optical images were exhibited in Figure S3. THF induced crystals are uniformly dispersed on wafer while DCM induced crystals gather together in one region with immature crystals around well-grown spherulites. Besides, toluene induced crystals show normal size (10-50 μm) and extremely large size spherulites (>100 μm). In contrast to aprotic solvents, 1-butanol induced crystals show Cupressaceae leaves-like structures.

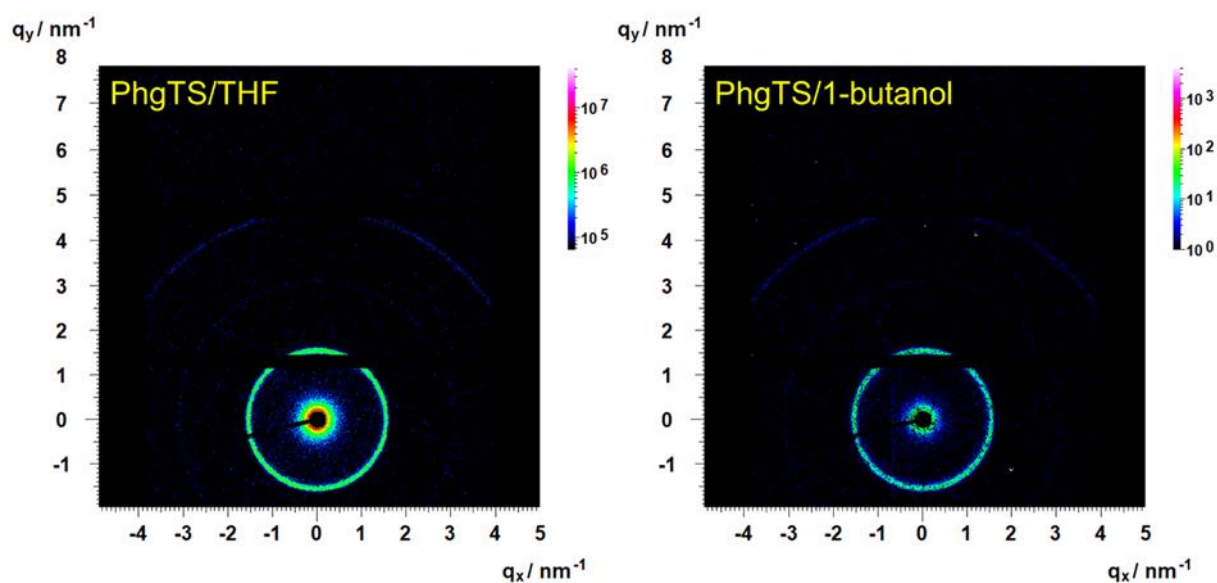


Figure S4. 2D SAXS-patterns of PhgTS crystals from THF and 1-butanol.

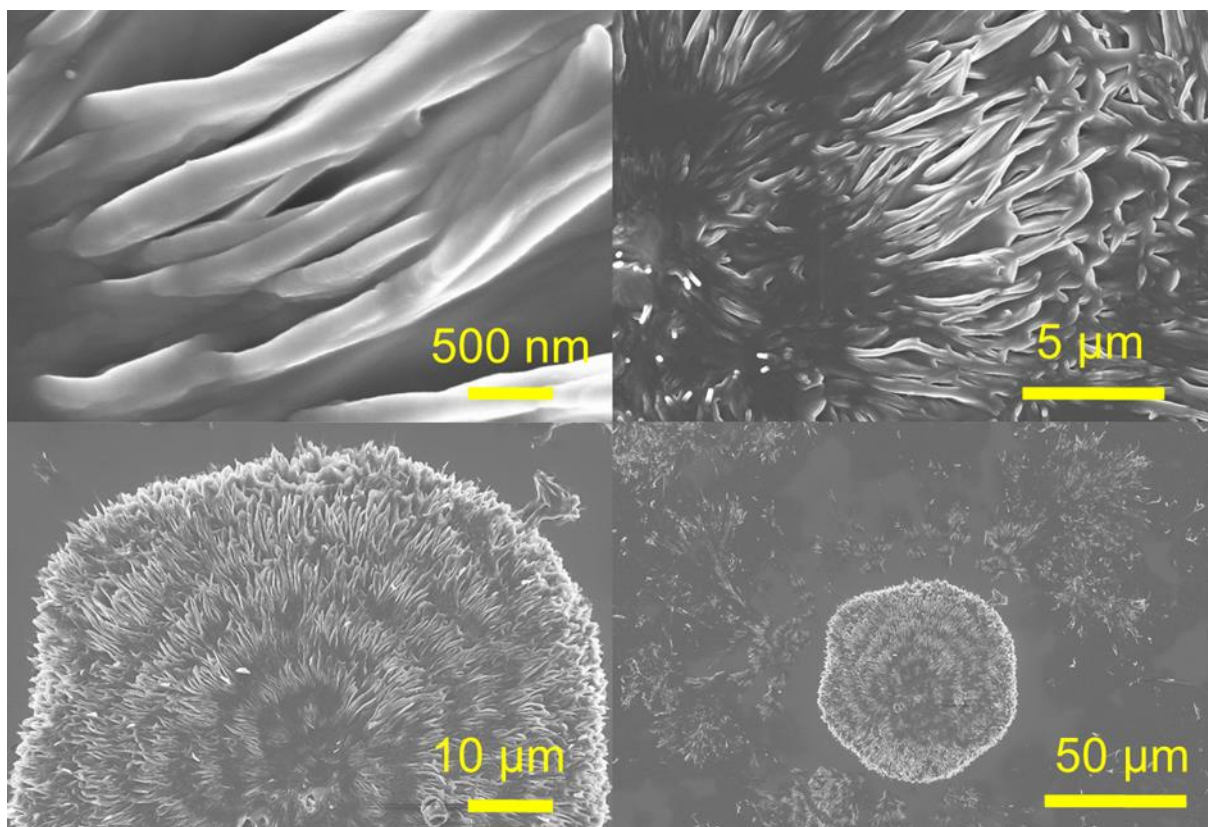


Figure S5. Zoom-in SEM images of PhgTS crystals induced by THF at 28°C with the concentration of 10 mg/mL.

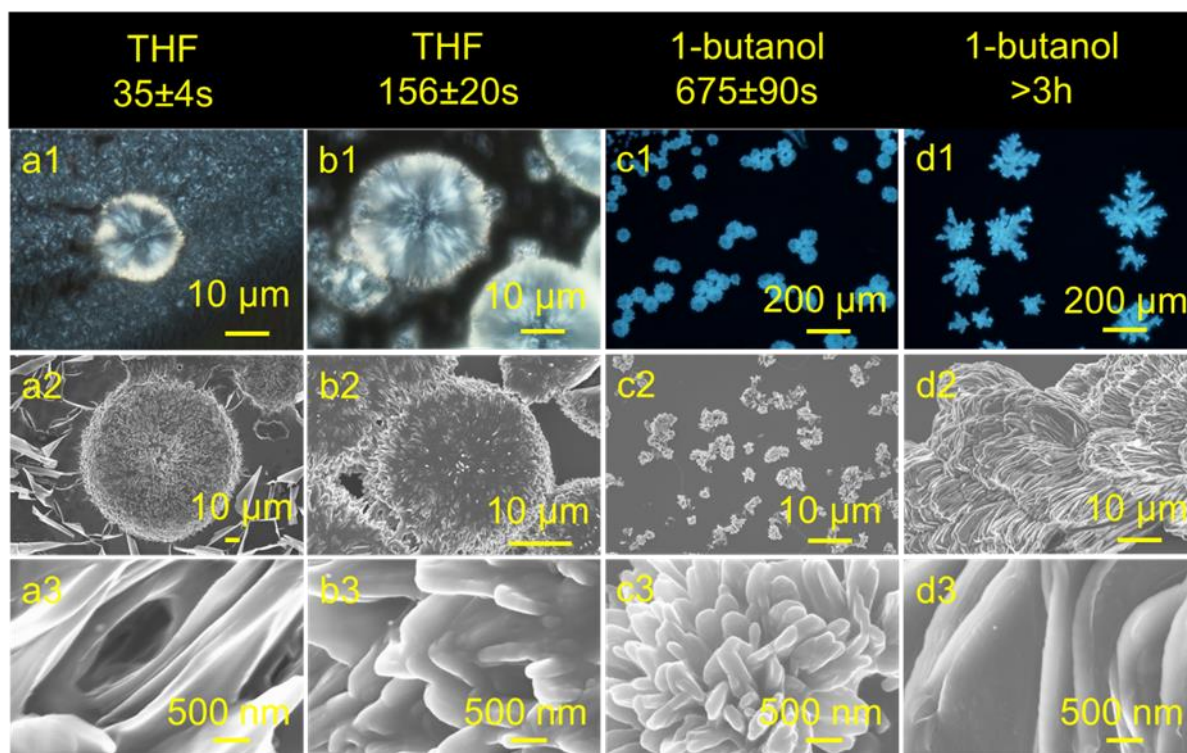


Figure S6. Morphologies of PhgTS crystals induced by THF and 1-butanol at 20°C with different evaporation time, the concentration is 10 mg/mL. (a1 and b1) Polarized optical microscope images of PhgTS crystals from THF with the evaporation time of 35 ± 4 s and 156 ± 20 s, respectively (c1 and d1) Polarized optical microscope images of PhgTS crystals from 1-butanol with the evaporation time of 675 ± 90 s and more than 3h (a2-d2) and (a3-d3) SEM images of PhgTS crystals in distinct magnifications.

The evaporation rates of solvents also have an influence on the morphology of PhgTS crystals as shown in Figure S6. With high evaporation rate of THF (Figure S6a1-S6a3), PhgTS crystals tend to form more hollow structures on the surface of spherulites (Figure S6b1-S6b3). For PhgTS crystals induced by 1-butanol, high evaporation rate (Figure S6c1-S6c3) led to smaller crystals. The morphology of these crystals is more bush-like instead of branch-like, comparing to the typical branch-like crystals from low evaporation rate (Figure S6d1-S6d3).