

Supplementary information for manuscript:

Pseudo-polymorphism in the toluene solvate of *p*-tert-butylcalix[5]arene: Structural and gas sorption investigations

As it was pointed out that the OH positions in reference [4] of the manuscript are incorrect, this has been resolved and is submitted as supporting information for the current manuscript.

Crystal data for TBC5·Tol I (original CSD entry DEVSAZ): C₁₃₈H₁₇₂O₁₀, *M* = 1990.76, triclinic, *a* = 17.127(3), *b* = 18.127(3), *c* = 22.045(3) Å, *α* = 87.057(3), *β* = 67.666(3), *γ* = 70.904(3)°, *U* = 5961.6(16) Å³, *μ* = 1.109 mm⁻¹, *T* = 173(2) K, space group *P*1, *Z* = 2, Mo-Kα radiation (wavelength *λ* = 0.71073 Å), final goodness of fit = 1.048, agreement index *R*₁ = 0.0788, 42944 reflections measured, 25654 unique (*R*_{int} = 0.0236) which were used in all calculations. The final weighted agreement index *ωR*(*F*²) was 0.2498 (all data).

Crystal data for Sublimed TBC5 (original CSD entry DEVSED): C_{27.50}H₃₅O_{2.5}, *M* = 405.55, orthorhombic, *a* = 12.780(3), *b* = 15.035(6), *c* = 15.340(4) Å, *U* = 4908(2) Å³, *μ* = 1.098 mm⁻¹, *T* = 173(2) K, space group *Pnma*, *Z* = 8, Mo-Kα radiation (wavelength *λ* = 0.71073 Å), final goodness of fit = 1.058, *R*₁ = 0.0911, 12069 reflections measured, 3610 unique (*R*_{int} = 0.1290) which were used in all calculations. The final *ωR*(*F*²) was 0.1992 (all data).