Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Hexameric assembly of 5,17-di-substituted calix[4]arene in the solid state

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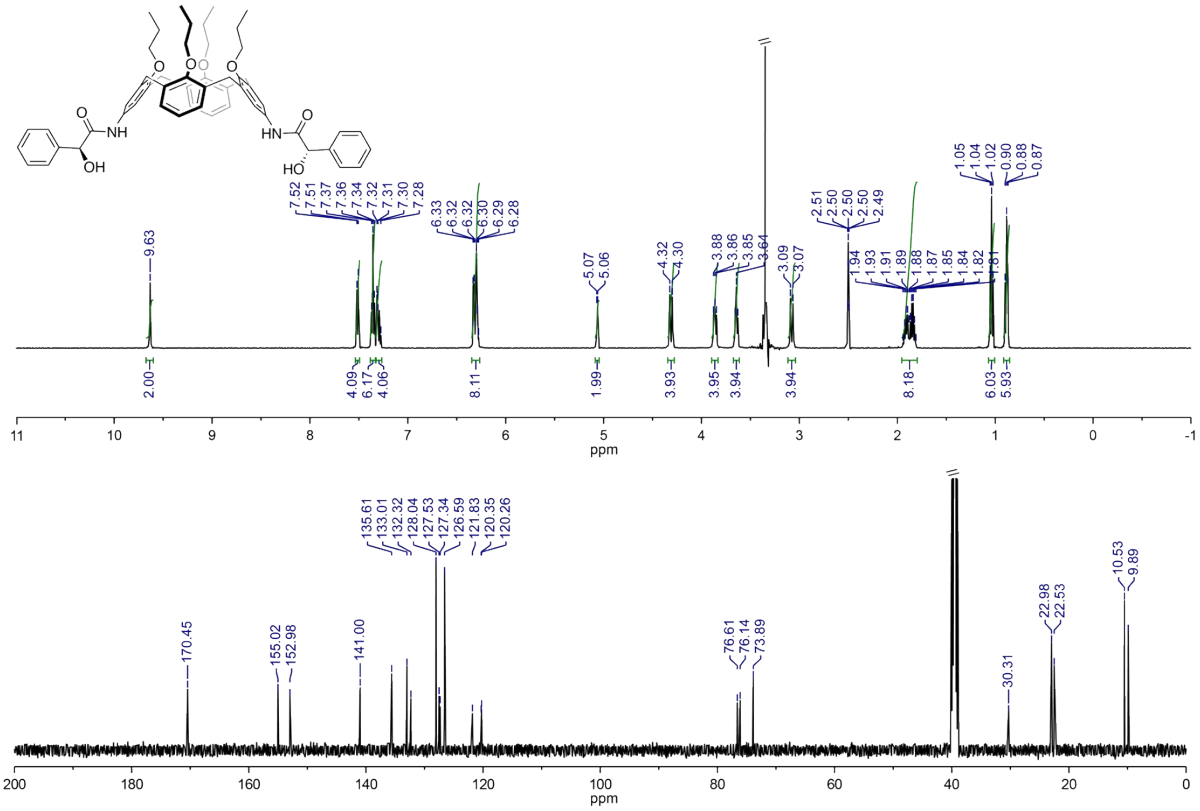

Figure S1. ^{1}H (500 MHz, DMSO-d_6, 293 K) and ^{13}C (125 MHz, DMSO-d_6, 293 K) NMR spectra of (*S*,*S*)-**1**.

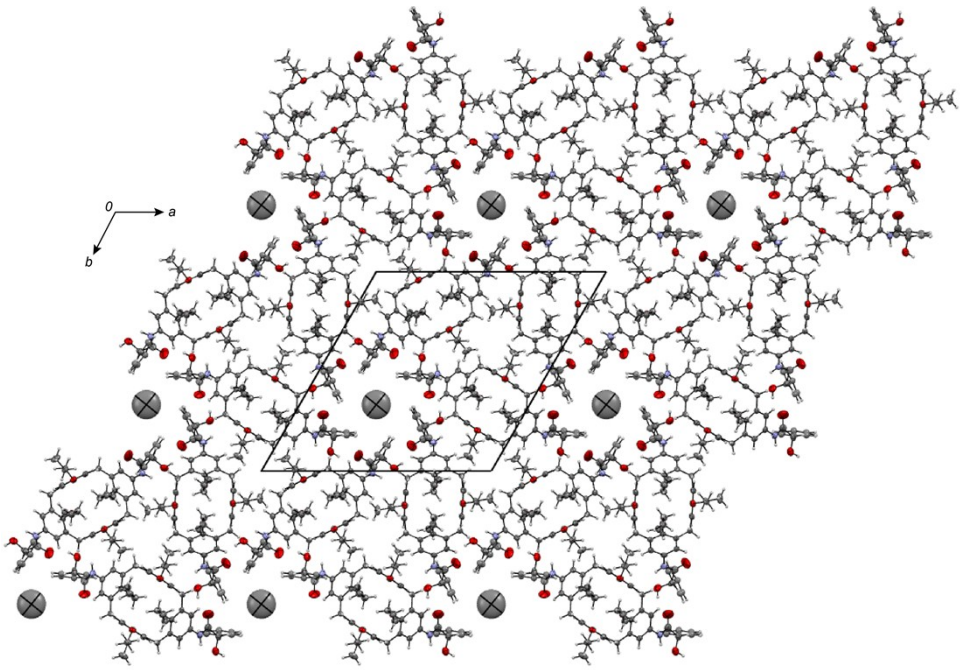

Figure S2. X-ray crystal structure of (*S*,*S*)-**1**·(MeOH) viewed down along the crystallographic *c* axis. Color scheme: gray (carbon), white (hydrogen), blue (nitrogen), red (oxygen).

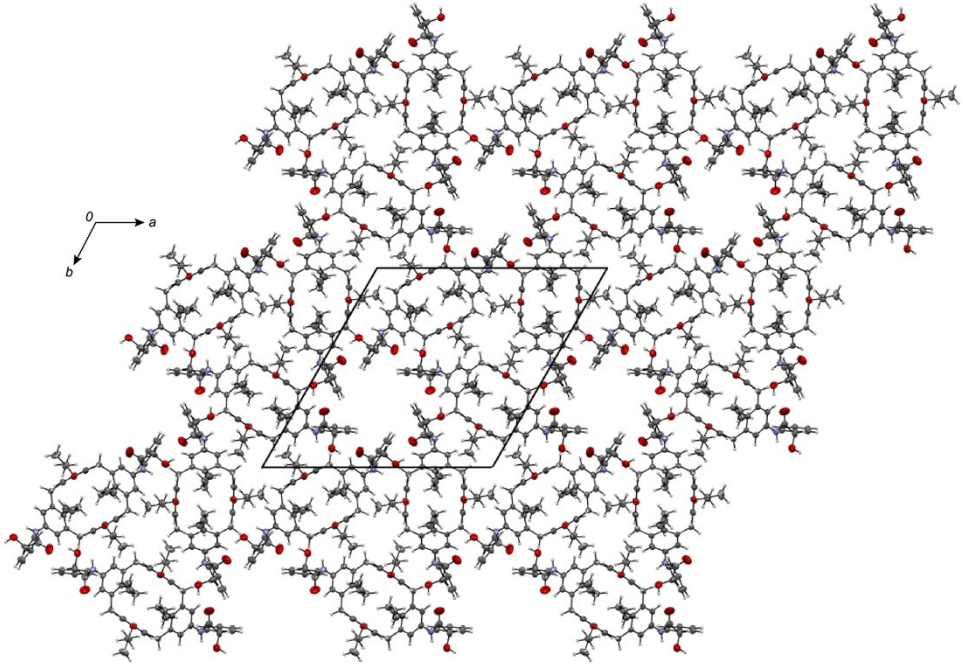

Figure S3. X-ray crystal structure of (*S*,*S*)-**1**·(1-PrOH) viewed down along the crystallographic *c* axis. Color scheme: gray (carbon), white (hydrogen), blue (nitrogen), red (oxygen).

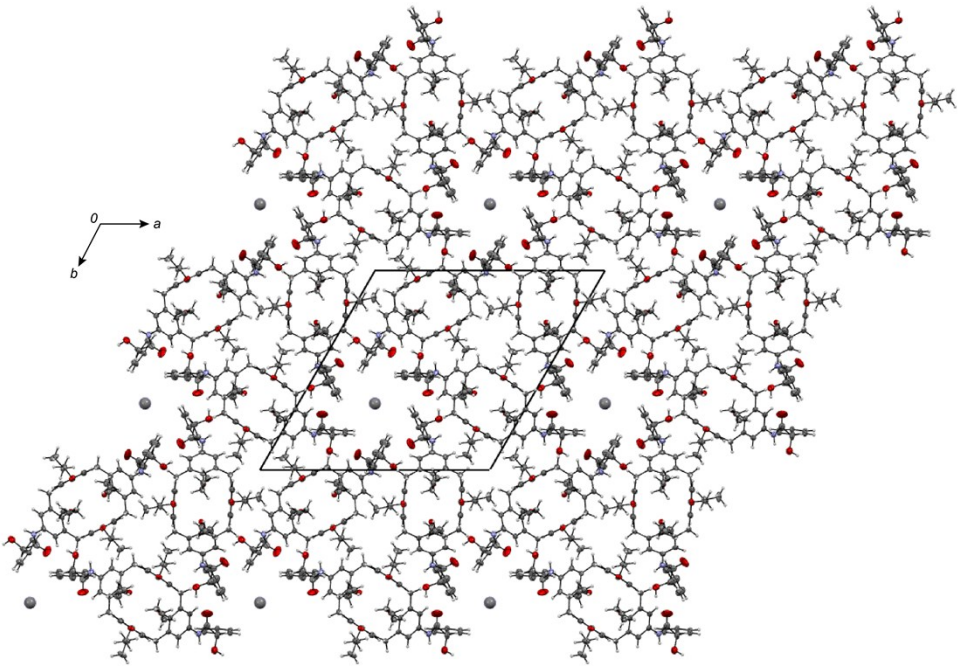

Figure S4. X-ray crystal structure of (*S*,*S*)-**1**·(CH_3CN) viewed down along the crystallographic *c* axis. Color scheme: gray (carbon), white (hydrogen), blue (nitrogen), red (oxygen).

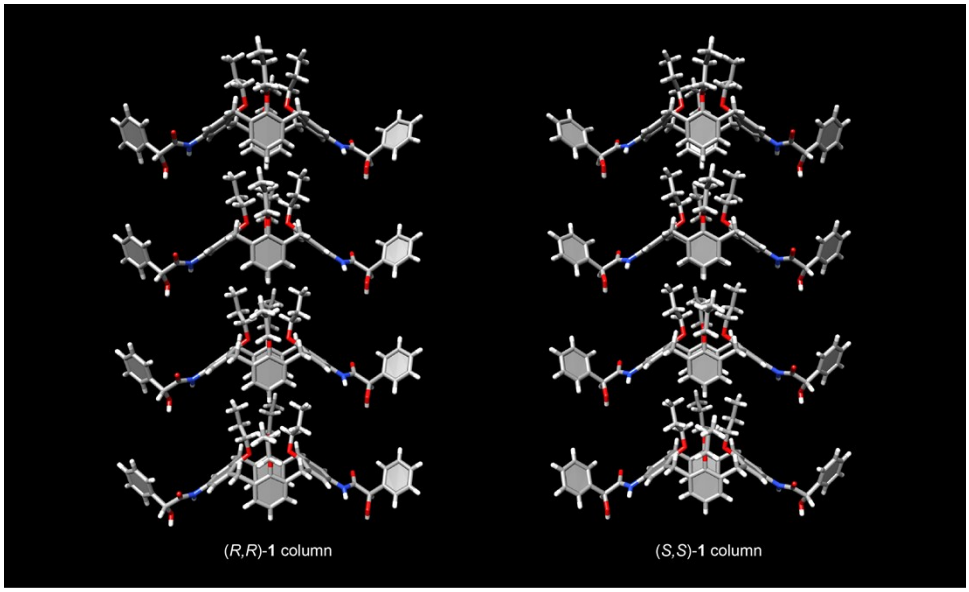

Figure S5. Head-to-tail columnar structures consisting of (*R*,*R*)-**1** (left) and (*S*,*S*)-**1** (right) found in *rac*-**1**. Color scheme: gray (carbon), white (hydrogen), blue (nitrogen), red (oxygen).

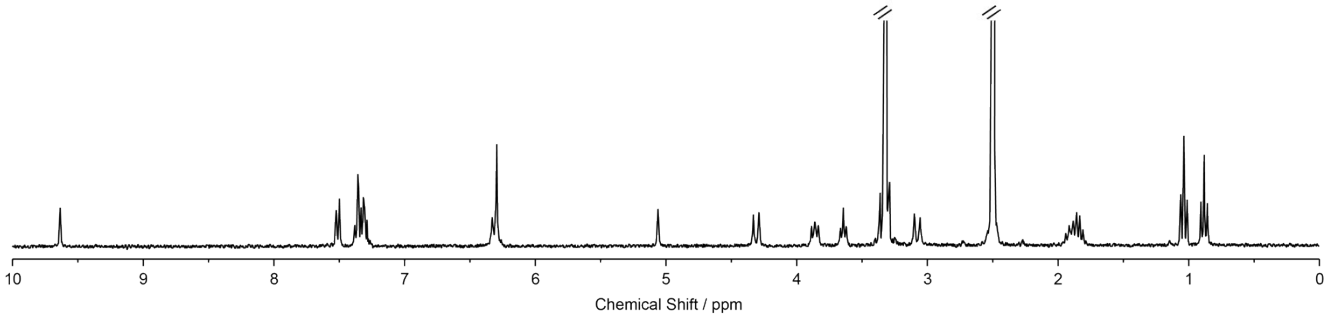

Figure S6. ^{1}H NMR spectrum (300 MHz, DMSO-d_6, 293 K) of (*S*,*S*)-**1**$_{apo}$.

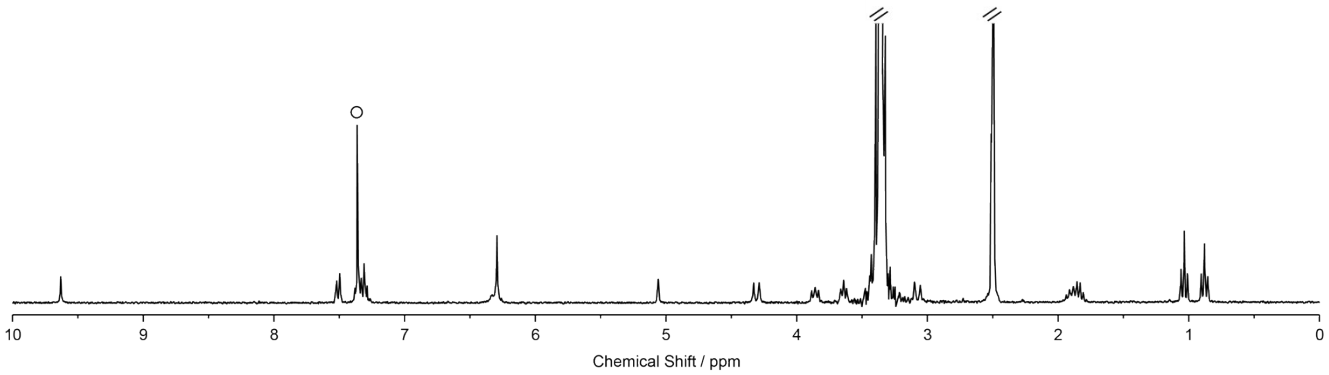

Figure S7. ^{1}H NMR spectrum (300 MHz, DMSO-d_6, 293 K) of (*S*,*S*)-**1**$_{apo}$ after contacting benzene vapor with (*S*,*S*)-**1**$_{apo}$ for 3 days at room temperature. Open circle denotes the signal of benzene.

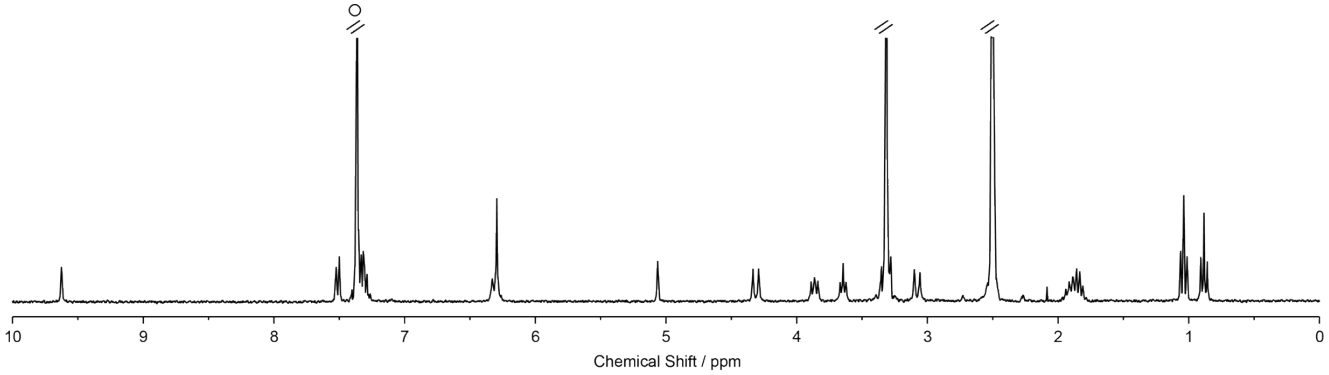

Figure S8. ^{1}H NMR spectrum (300 MHz, DMSO-d_6, 293 K) of (*S*,*S*)-**1**$_{apo}$ after contacting a mixed vapor of benzene and acetone with (*S*,*S*)-**1**$_{apo}$ for 3 days at room temperature. Open circle denotes the signal of benzene.

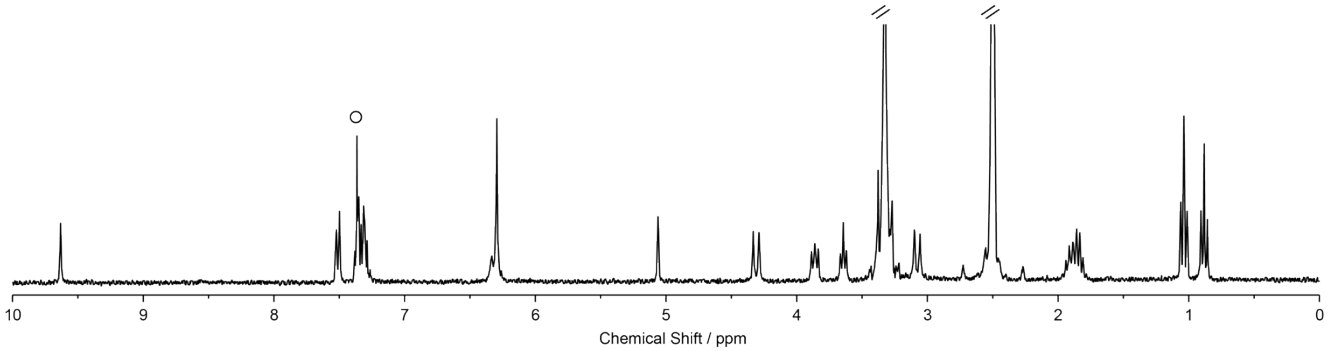

Figure S9. ^{1}H NMR spectrum (300 MHz, DMSO-d_6, 293 K) of (*S*,*S*)-**1**$_{apo}$ after contacting a mixed vapor of benzene and ethyl acetate with (*S*,*S*)-**1**$_{apo}$ for 3 days at room temperature. Open circle denotes the signal of benzene.