

Unusual Conformations of a Hexa-Host Molecule in Solvate Inclusion Compounds

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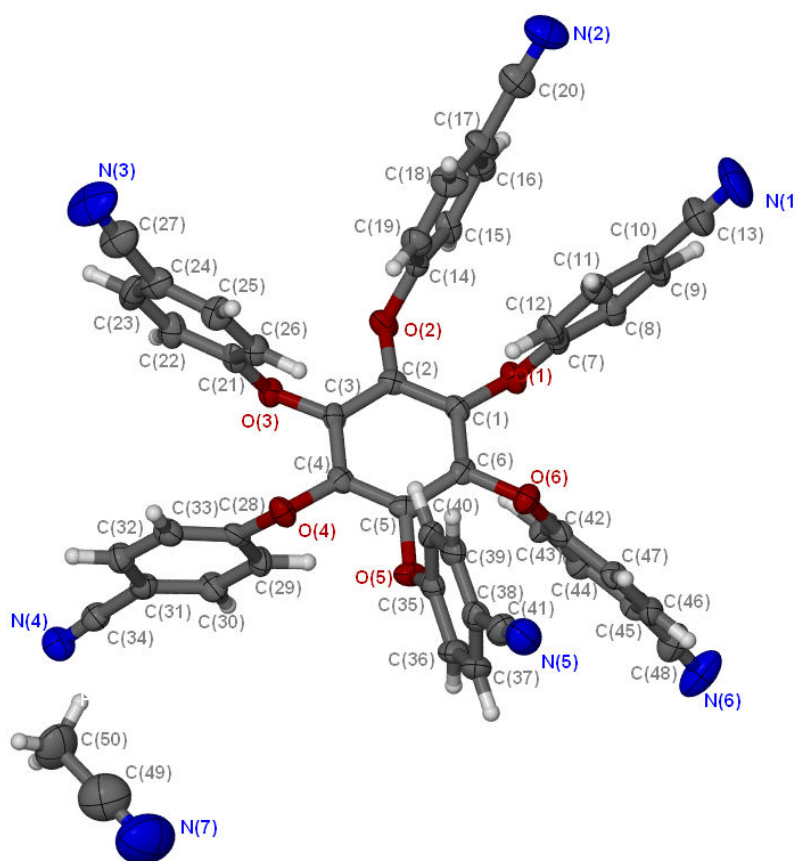


Figure S1. Thermal ellipsoid plot of **1a**. Atoms are shown with 70% probability thermal ellipsoids.

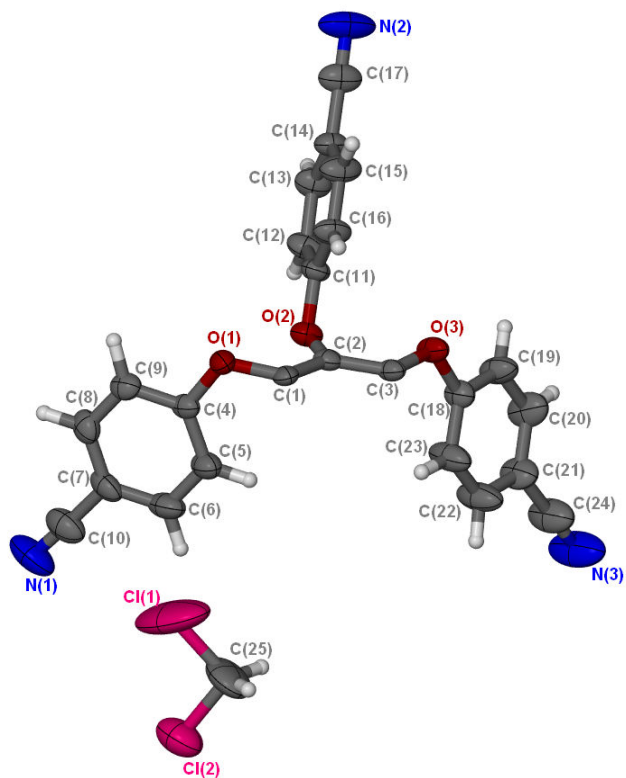


Figure S2. Thermal ellipsoid plot of **1b**. Atoms are shown with 70% probability thermal ellipsoids.

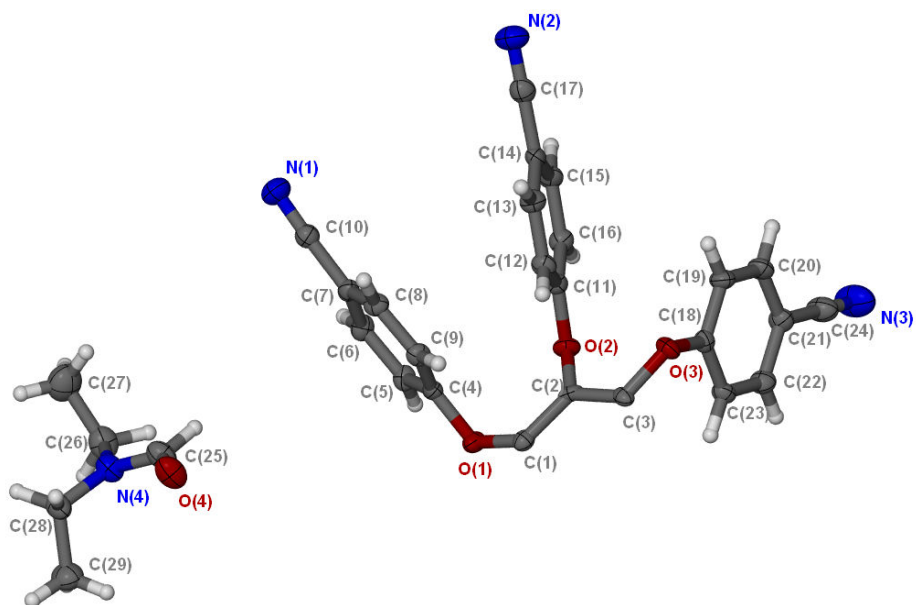


Figure S3. Thermal ellipsoid plot of **1c**. Atoms are shown with 70% probability thermal ellipsoids.

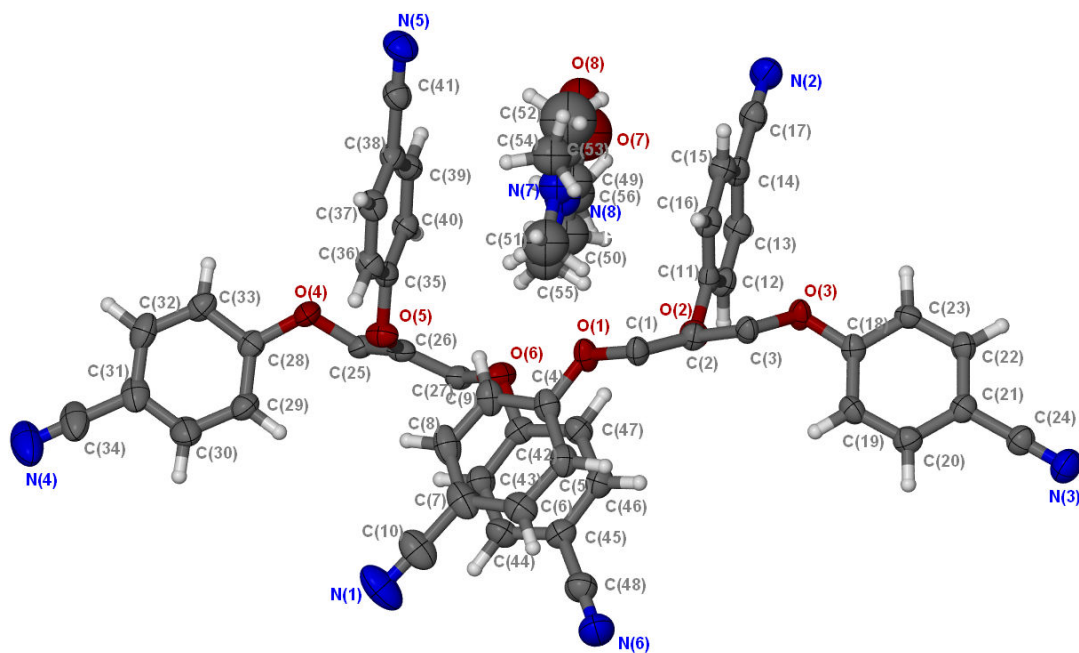


Figure S4. Thermal ellipsoid plot of **1d**. Atoms are shown with 70% probability thermal ellipsoids.

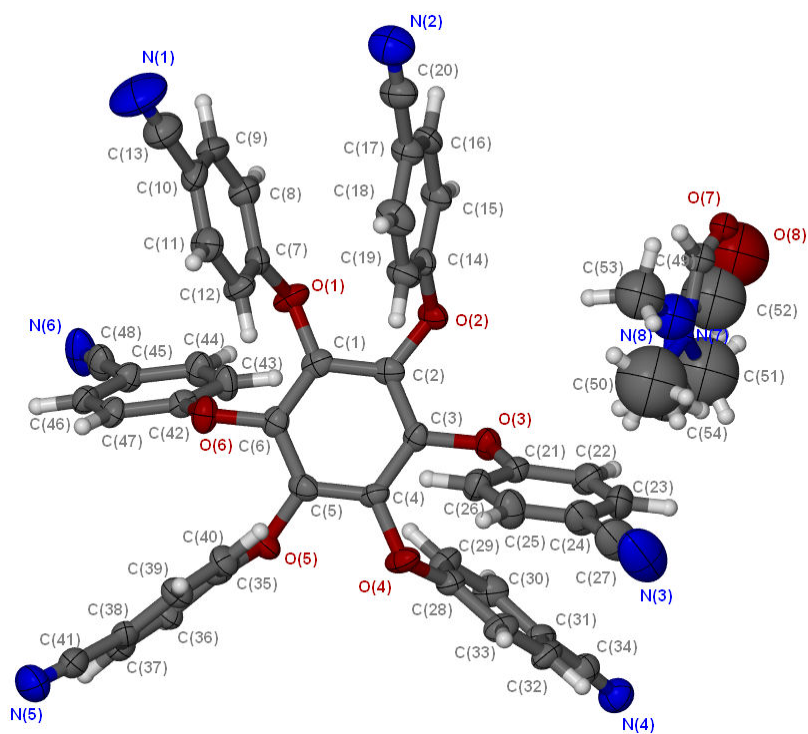


Figure S5. Thermal ellipsoid plot of **1e**. Atoms are shown with 70% probability thermal ellipsoids.

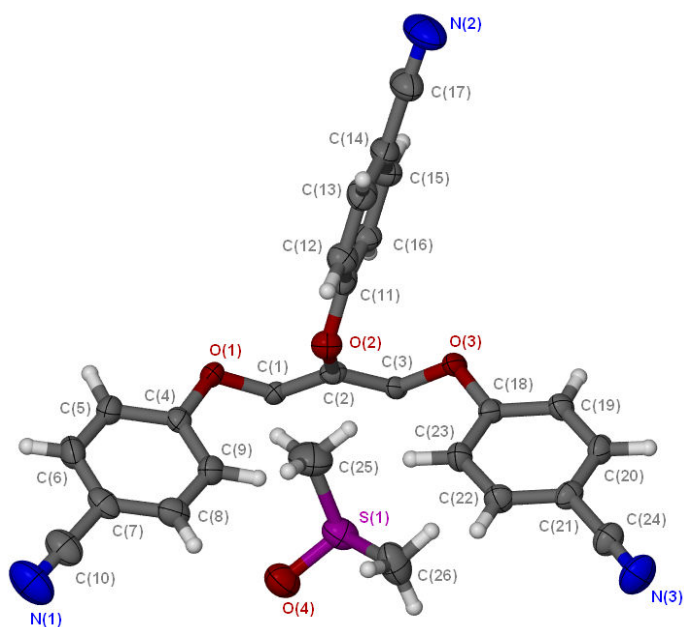


Figure S6. Thermal ellipsoid plot of **1f**. Atoms are shown with 70% probability thermal ellipsoids.

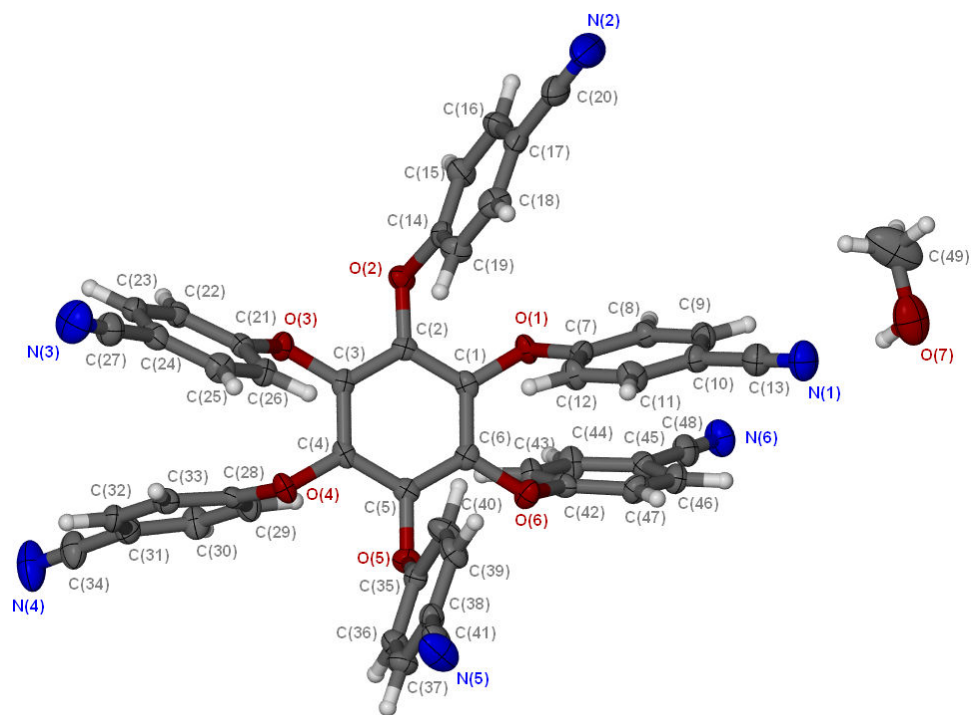


Figure S7. Thermal ellipsoid plot of **1g**. Atoms are shown with 70% probability thermal ellipsoids.

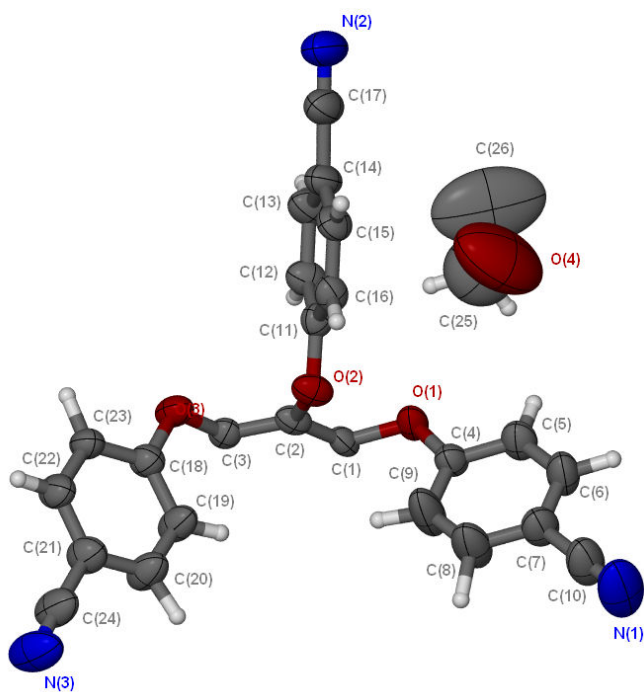


Figure S8. Thermal ellipsoid plot of **1h**. Atoms are shown with 70% probability thermal ellipsoids.

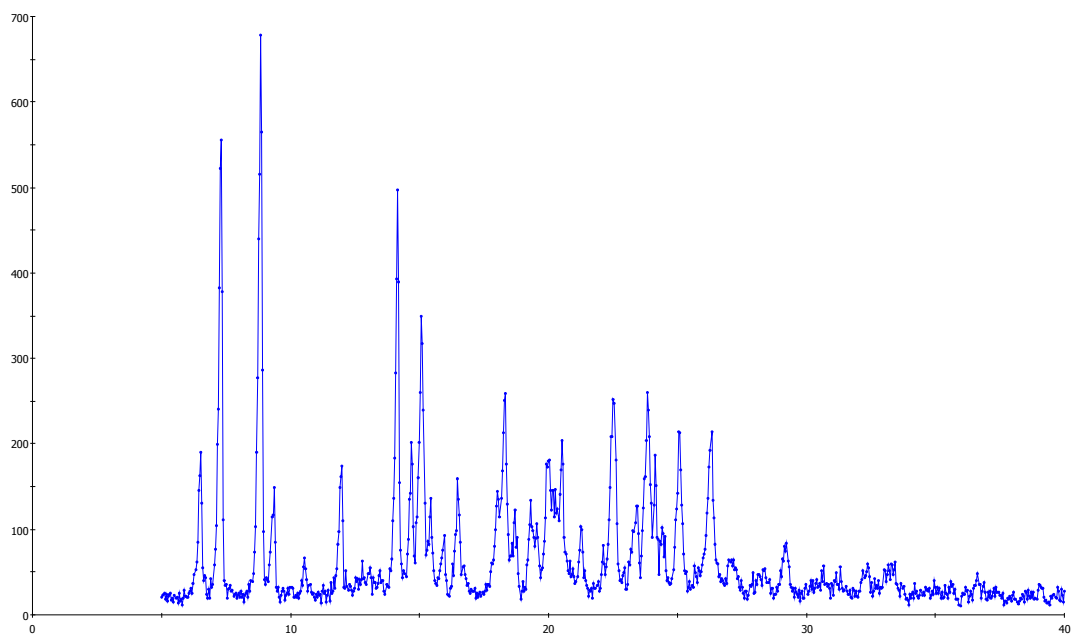


Figure S9. Experimental powder X-ray diffraction pattern of **1a**.

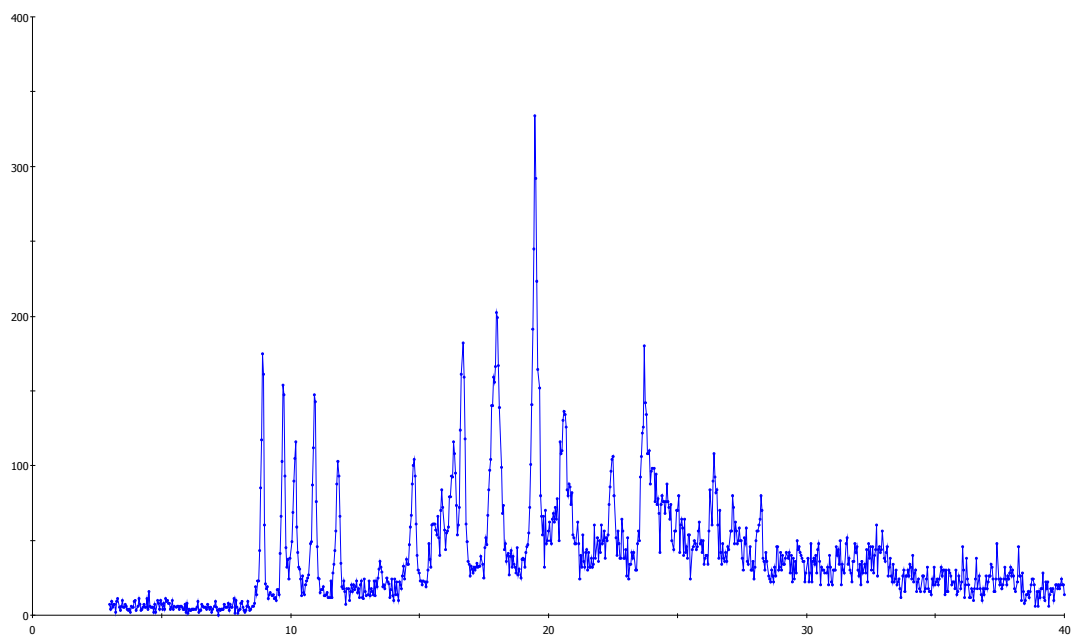


Figure S10. Experimental powder X-ray diffraction pattern of **1b**.

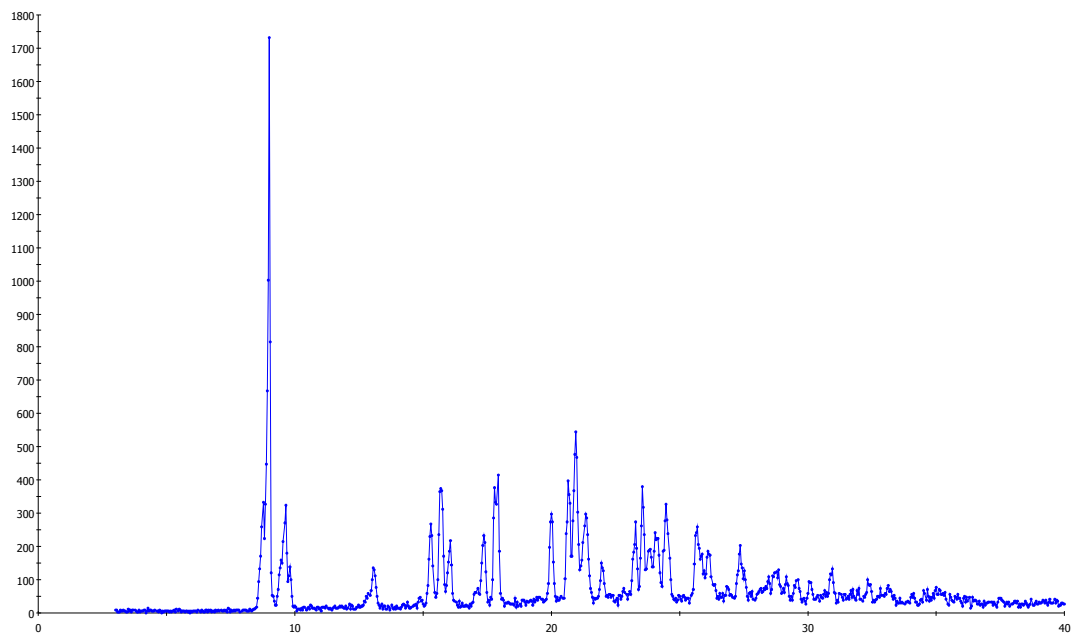


Figure S11. Experimental powder X-ray diffraction pattern of **1c**.

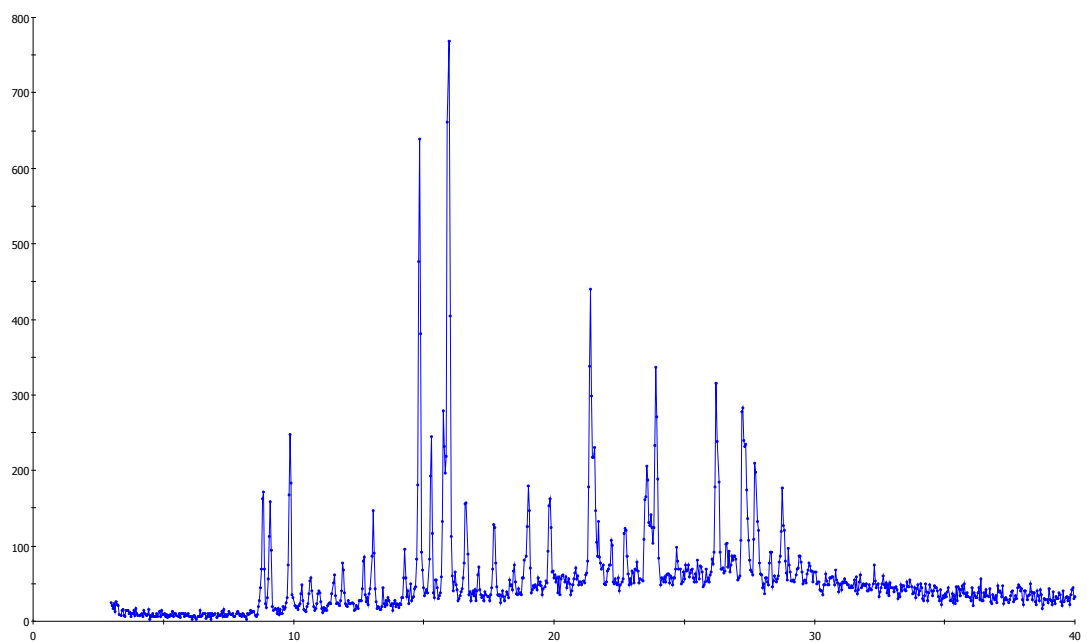


Figure S12. Experimental powder X-ray diffraction pattern of **1d**.

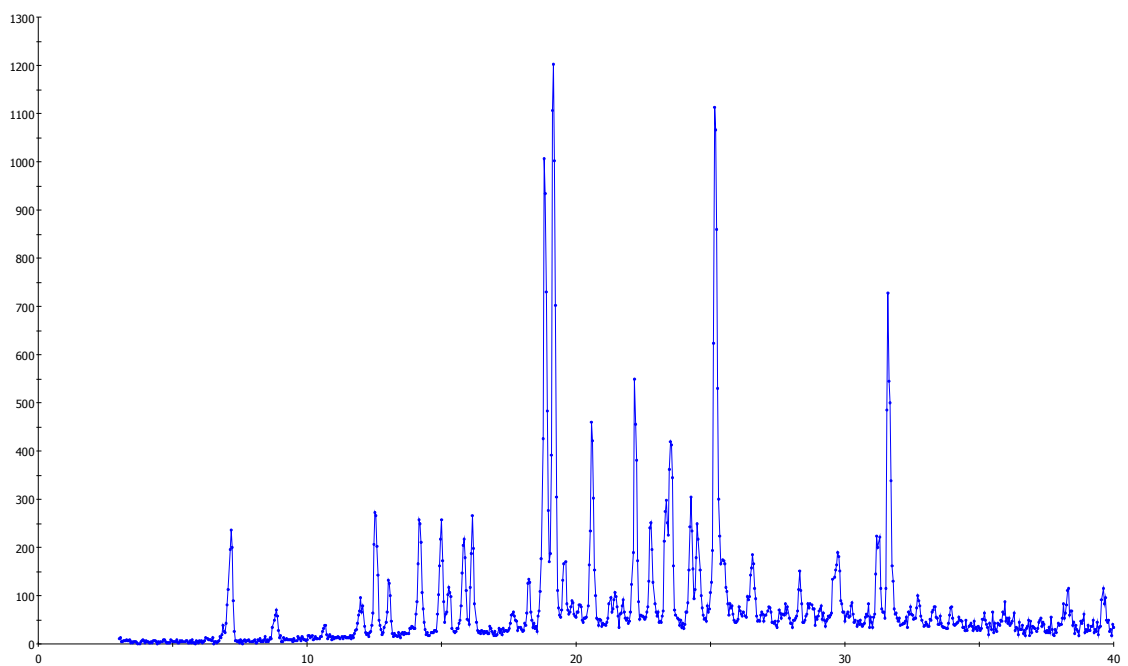


Figure S13. Experimental powder X-ray diffraction pattern of **1e**.

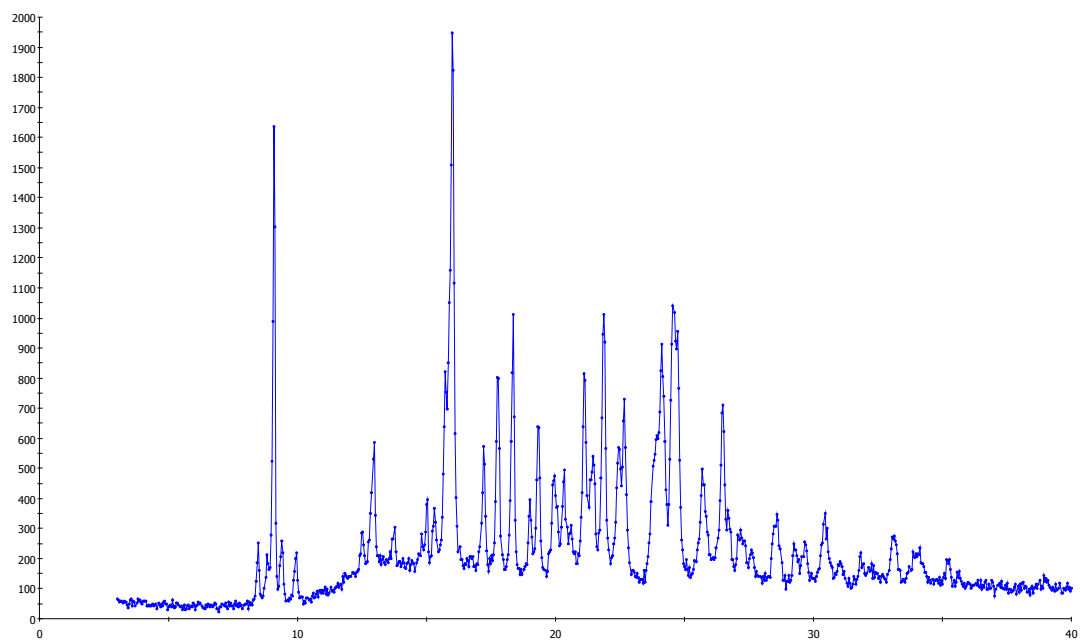


Figure S14. Experimental powder X-ray diffraction pattern of **1f**.

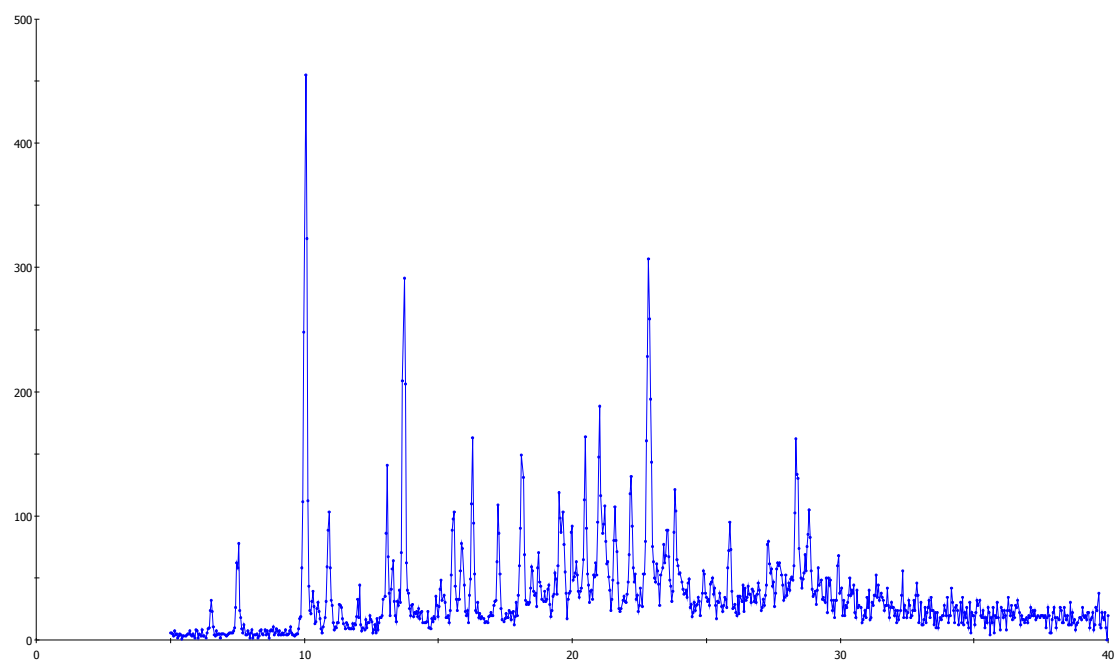


Figure S15. Experimental powder X-ray diffraction pattern of **1g**.

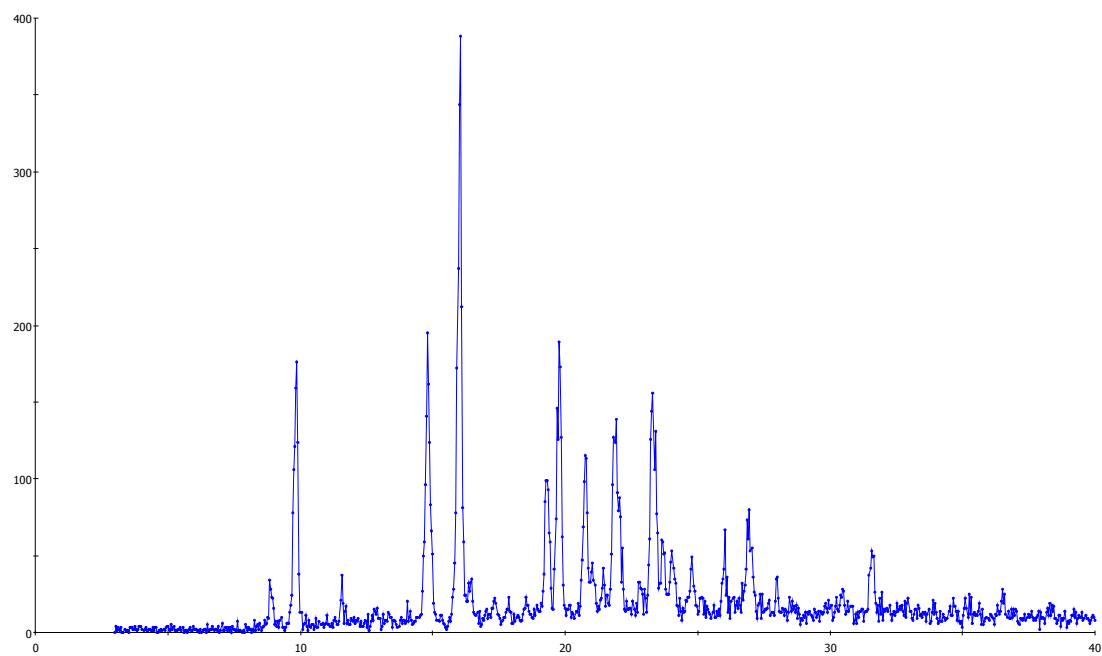


Figure S16. Experimental powder X-ray diffraction pattern of **1h**.

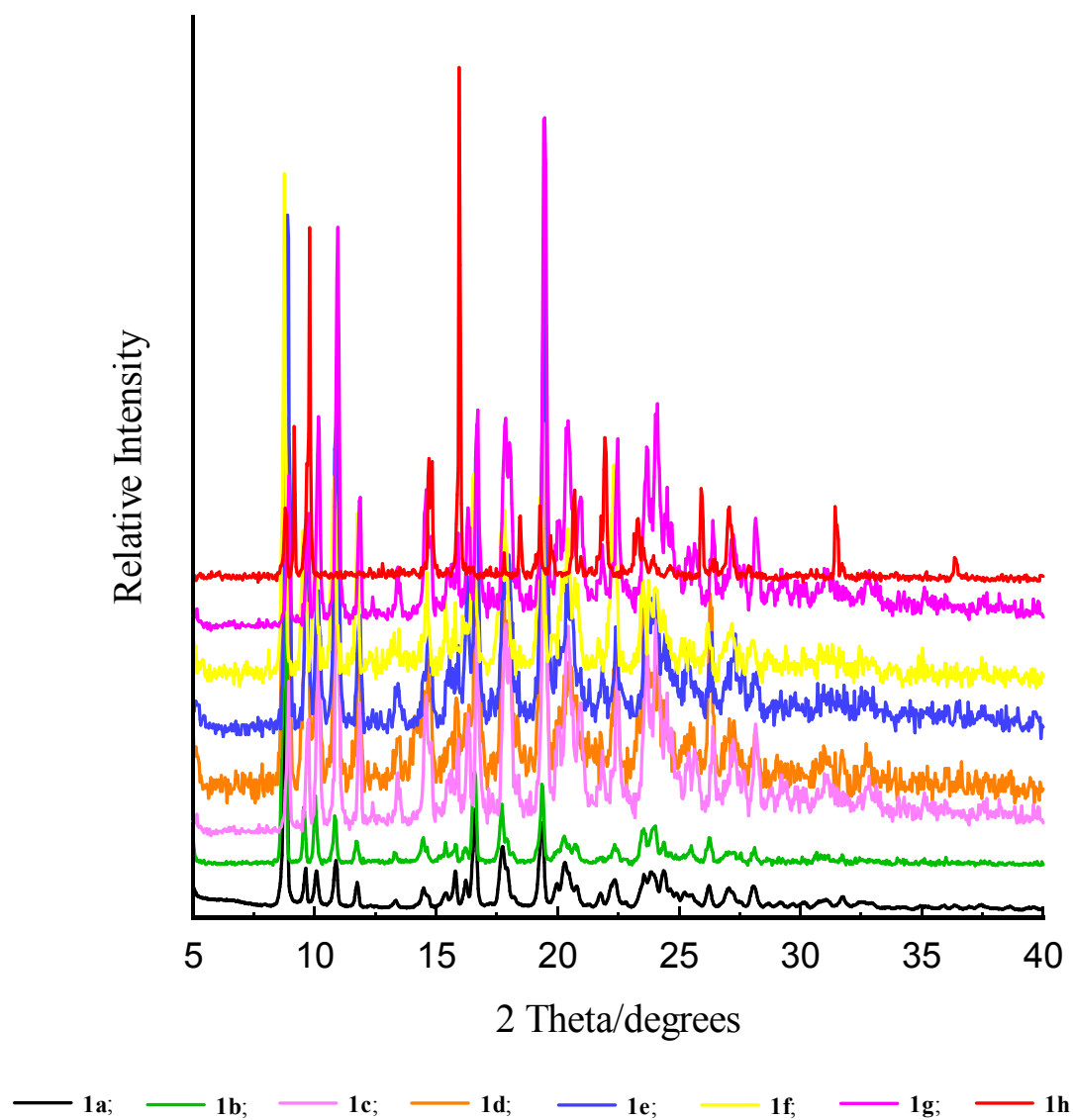


Figure S17. Experimental powder X-ray diffraction pattern of desolvated materials after heating at ca. 200 °C.

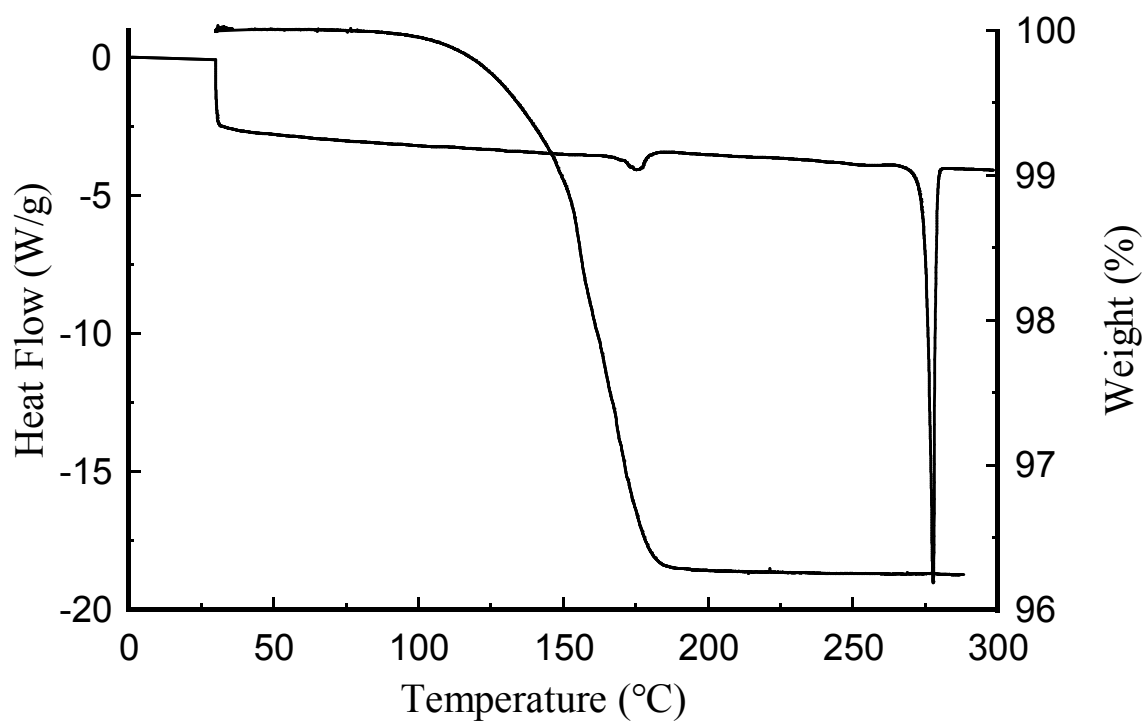


Figure S18.DSC and TGA thermogram of **1a**

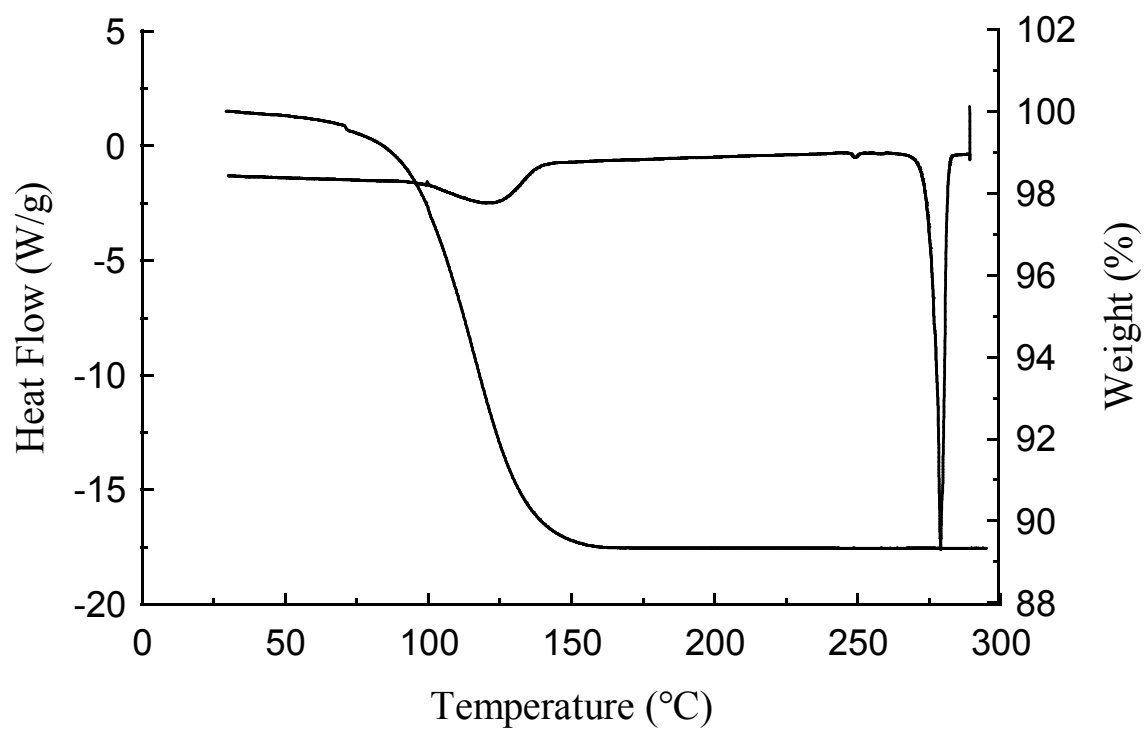


Figure S19.DSC and TGA thermogram of **1b**

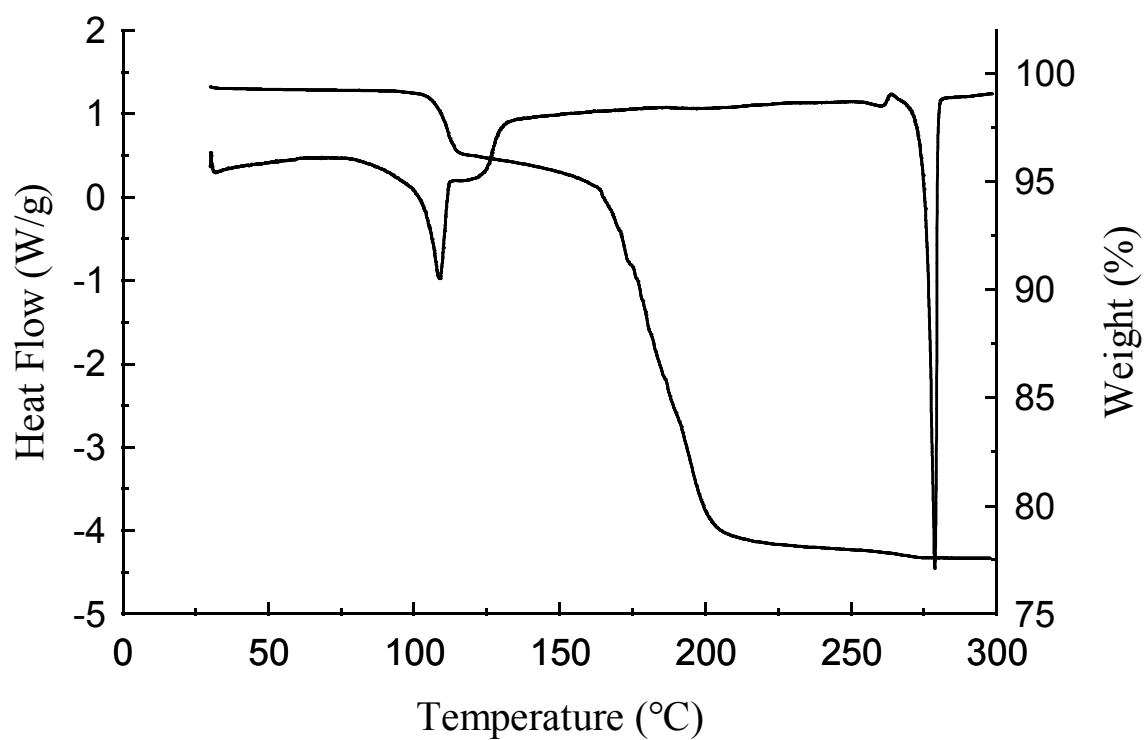


Figure S20.DSC and TGA thermogram of **1c**

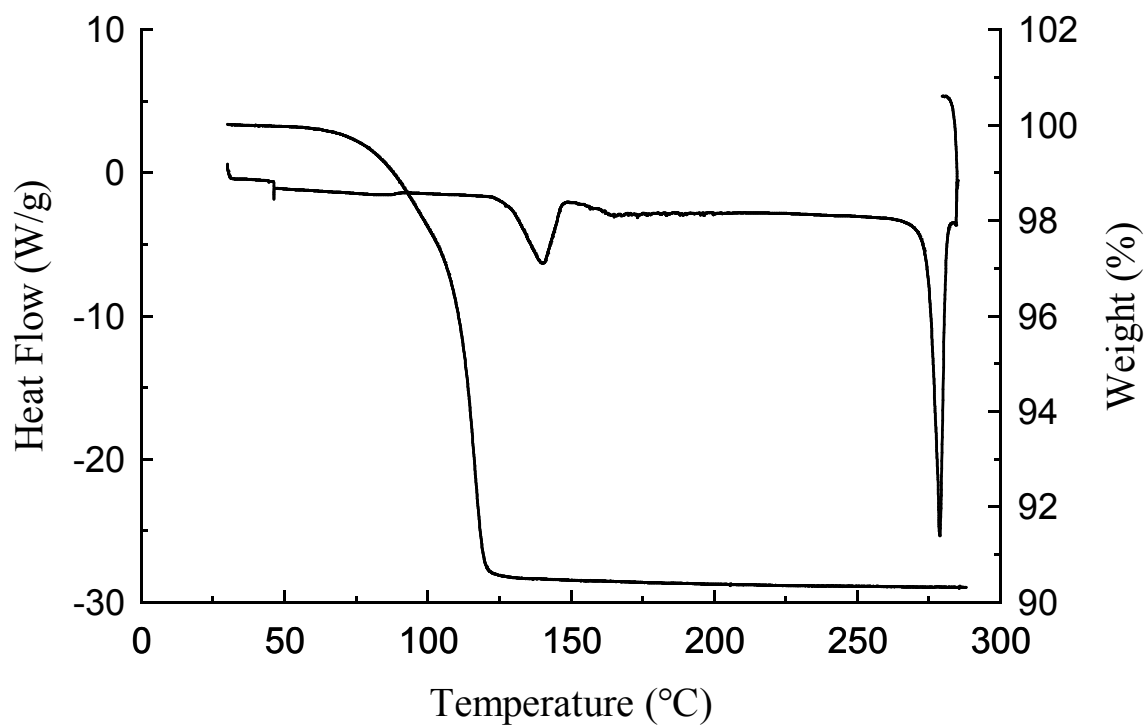


Figure S21.DSC and TGA thermogram of **1d**

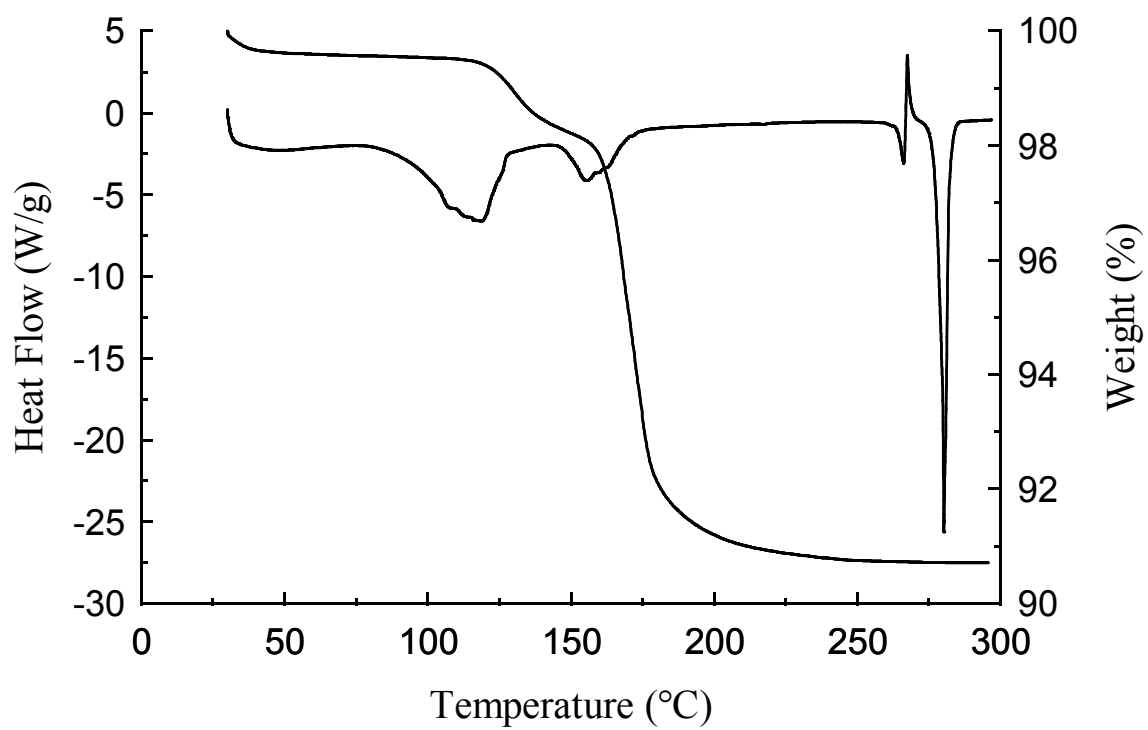


Figure S22.DSC and TGA thermogram of **1e**

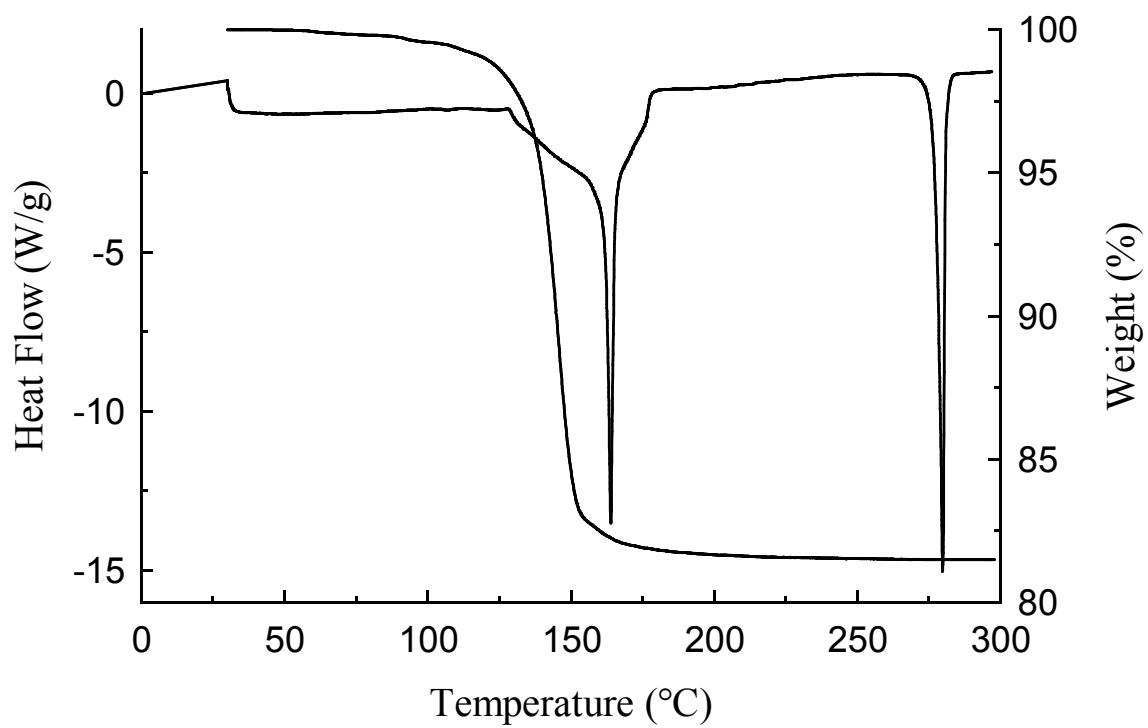


Figure S23.DSC and TGA thermogram of **1f**

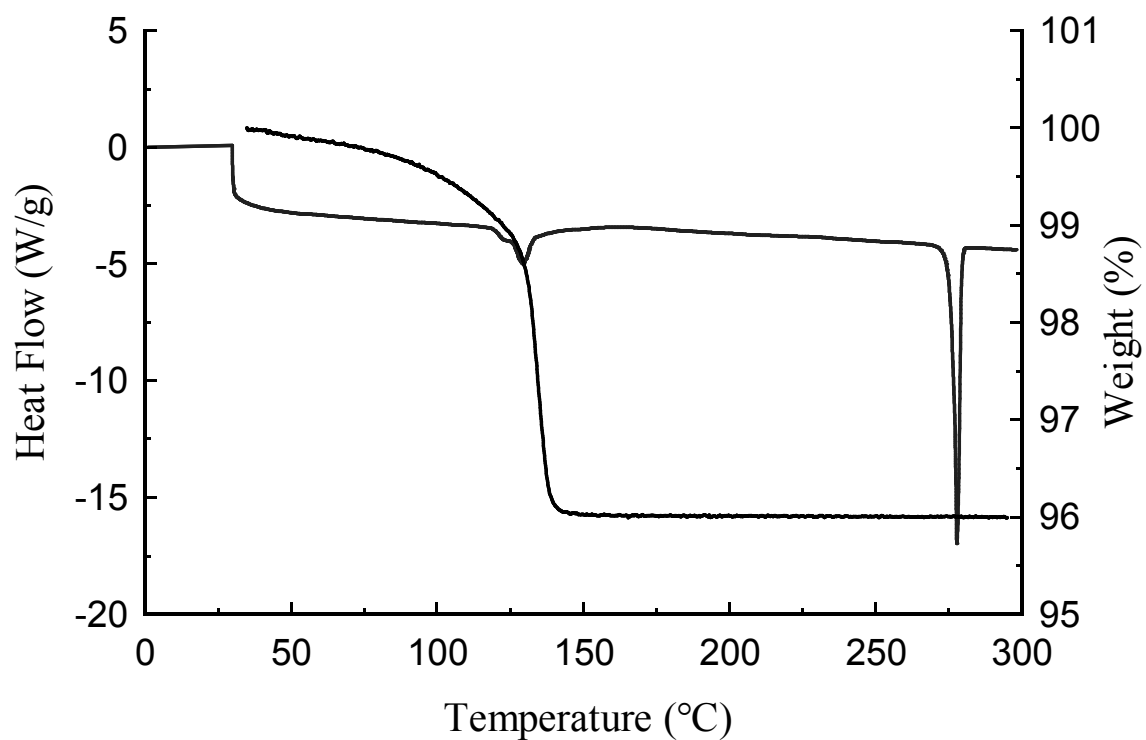


Figure S24.DSC and TGA thermogram of **1g**

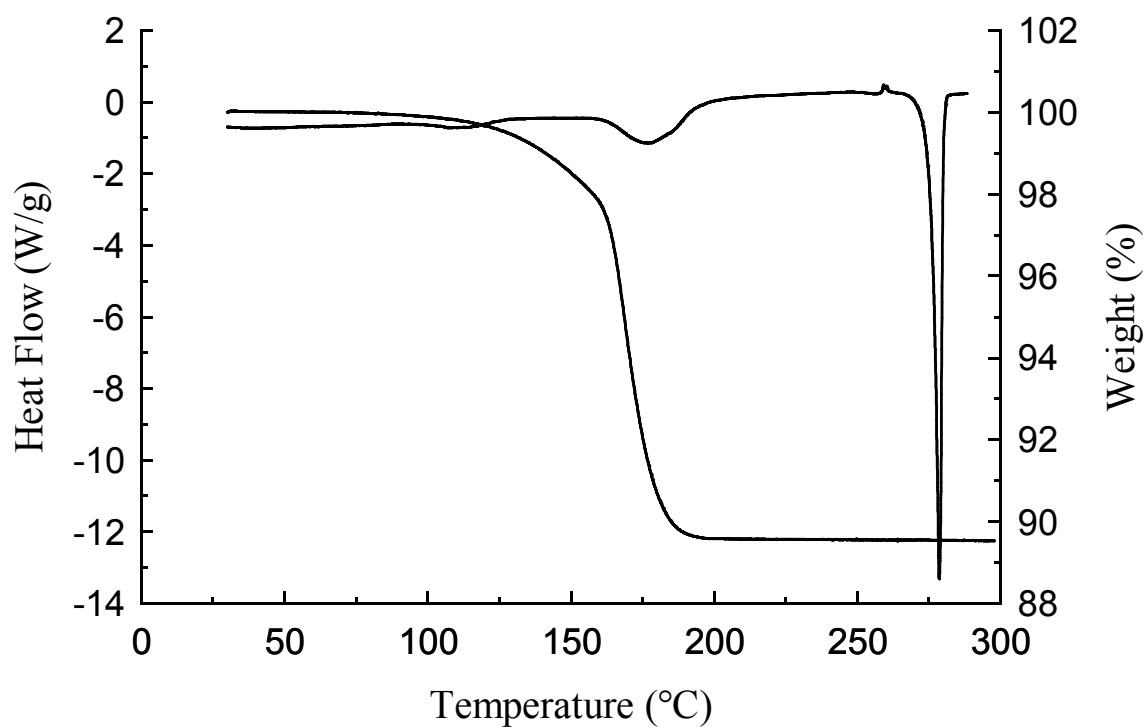


Figure S25.DSC and TGA thermogram of **1h**

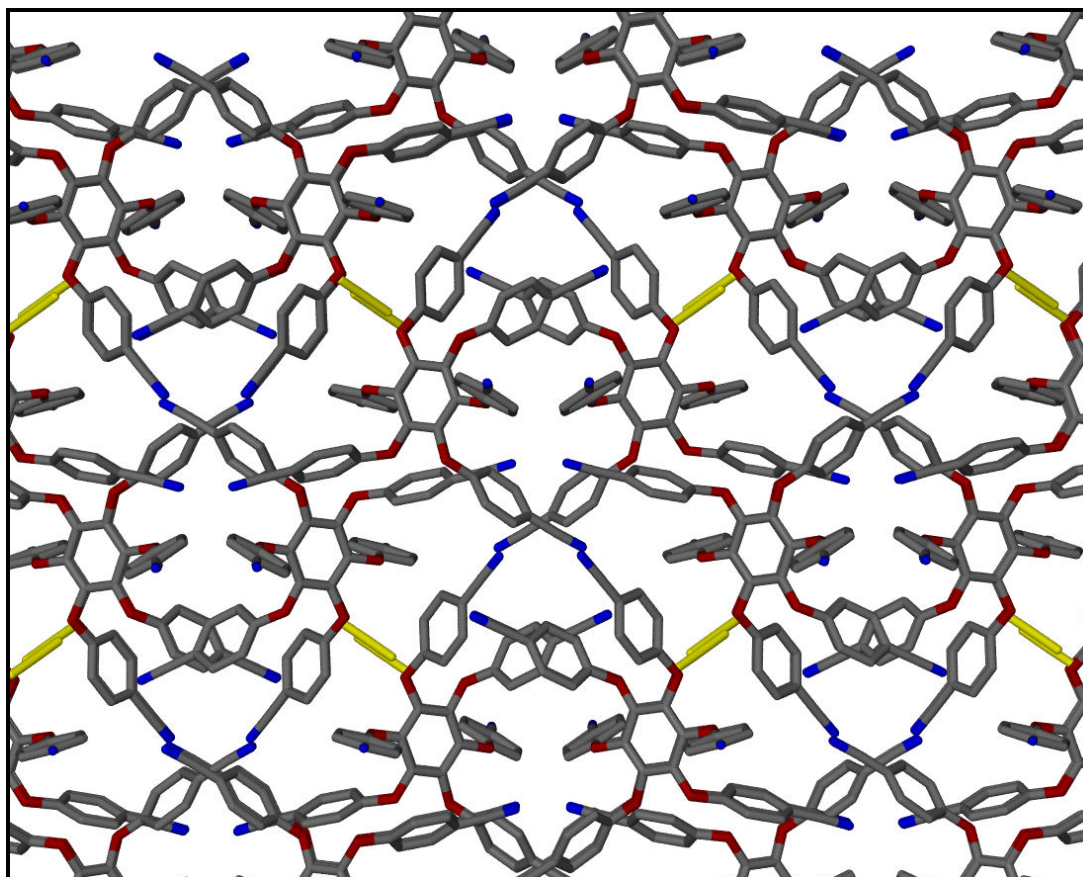


Figure S26. Packing diagram of **1a**, viewed along the *b* axis. Hydrogen atoms are omitted for clarity. Acetonitrile molecules are shown in yellow.

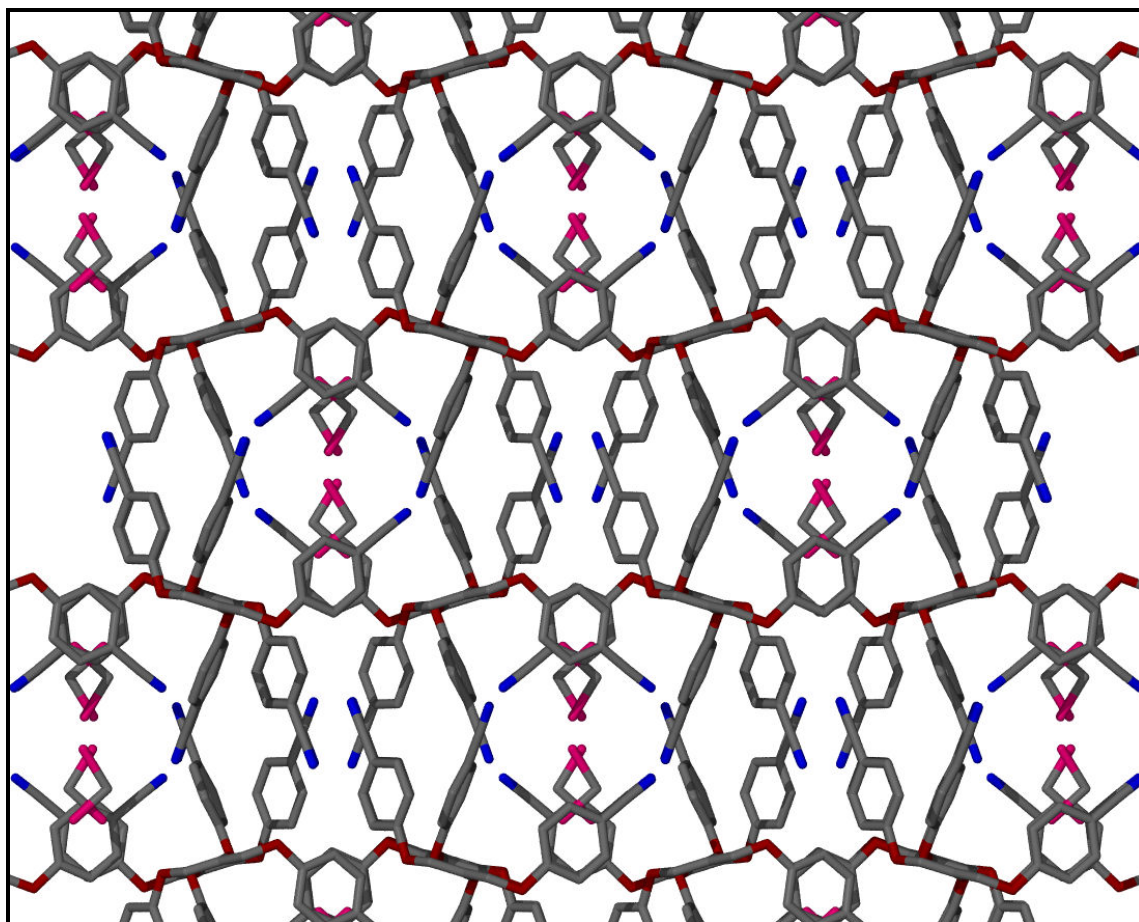


Figure S27. Packing diagram of **1b**, viewed along the *c* axis. Hydrogen atoms are omitted for clarity.

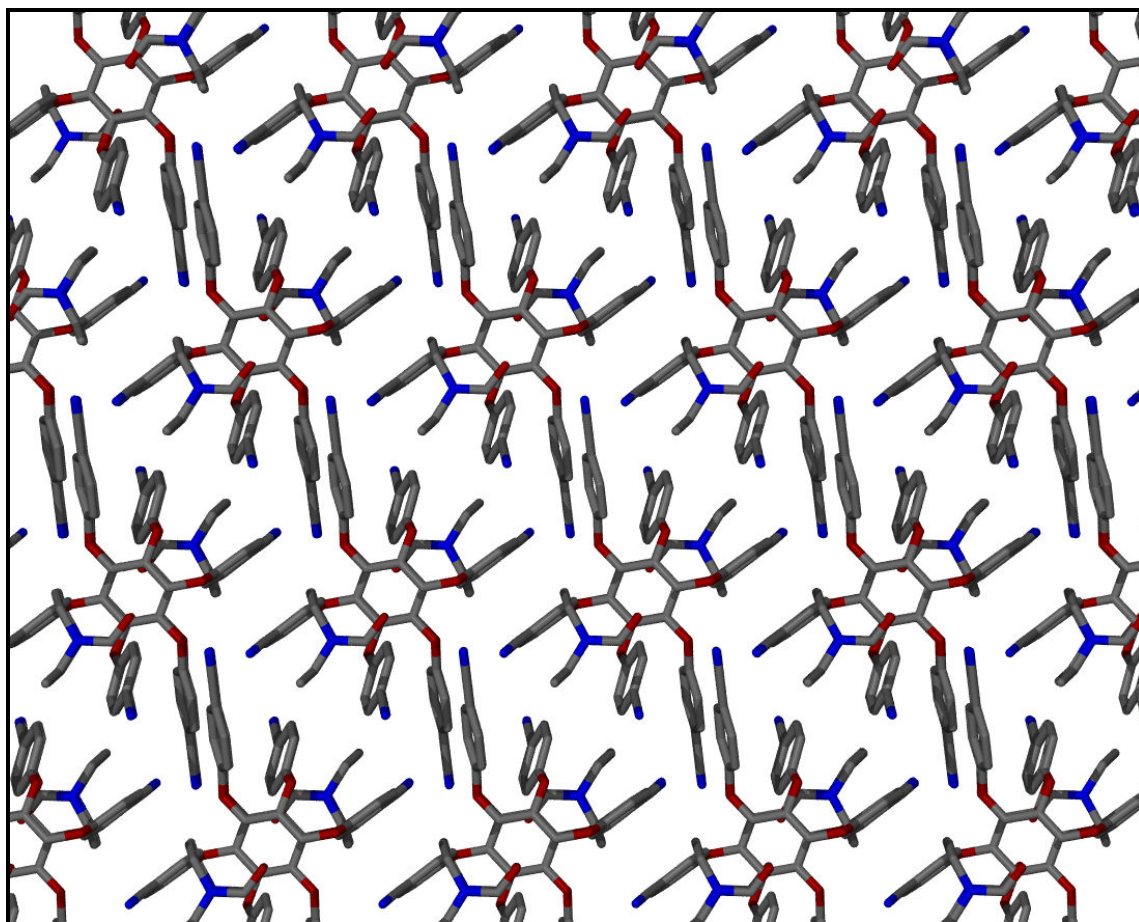


Figure S28. Packing diagram of **1c**, viewed along the *c* axis. Hydrogen atoms are omitted for clarity.

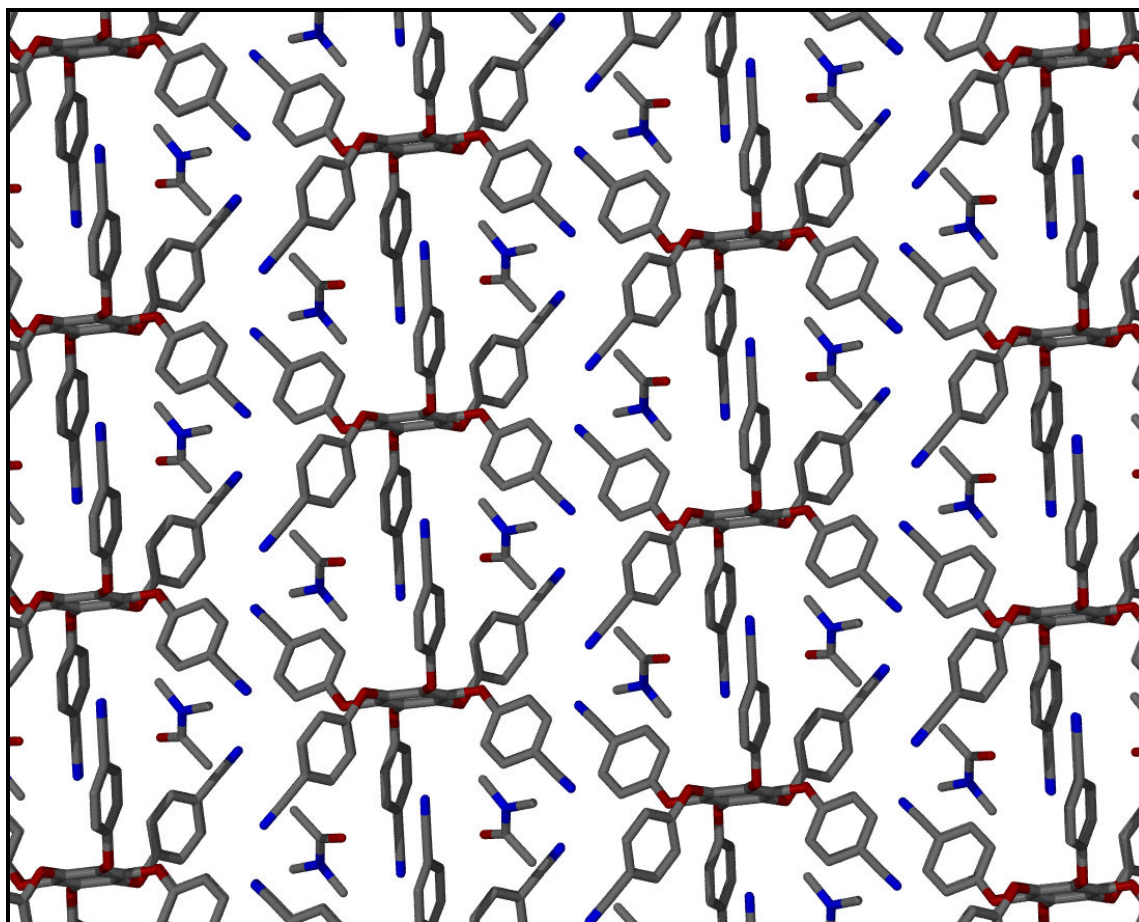


Figure S29. Packing diagram of **1d**, viewed along the *a* axis. Hydrogen atoms are omitted for clarity.

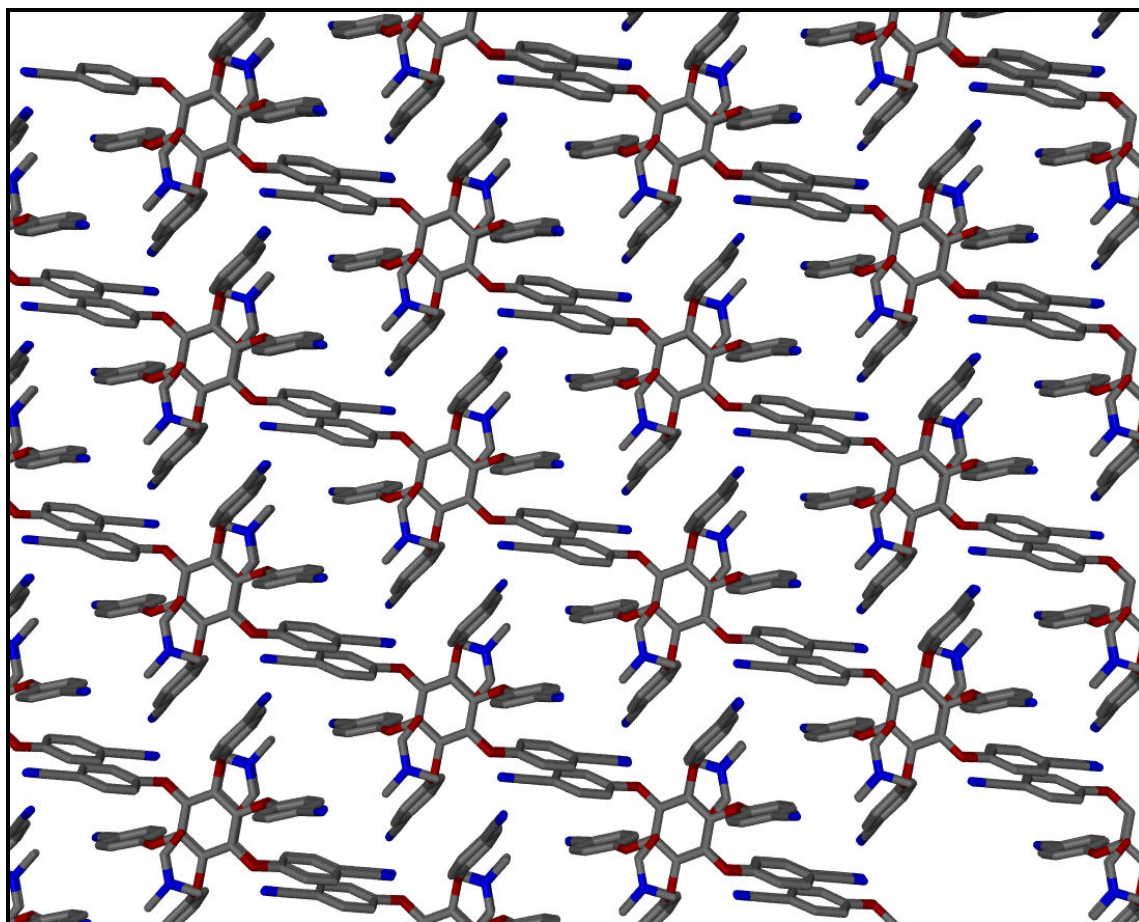


Figure S30. Packing diagram of **1e**, viewed along the *b* axis. Hydrogen atoms are omitted for clarity.

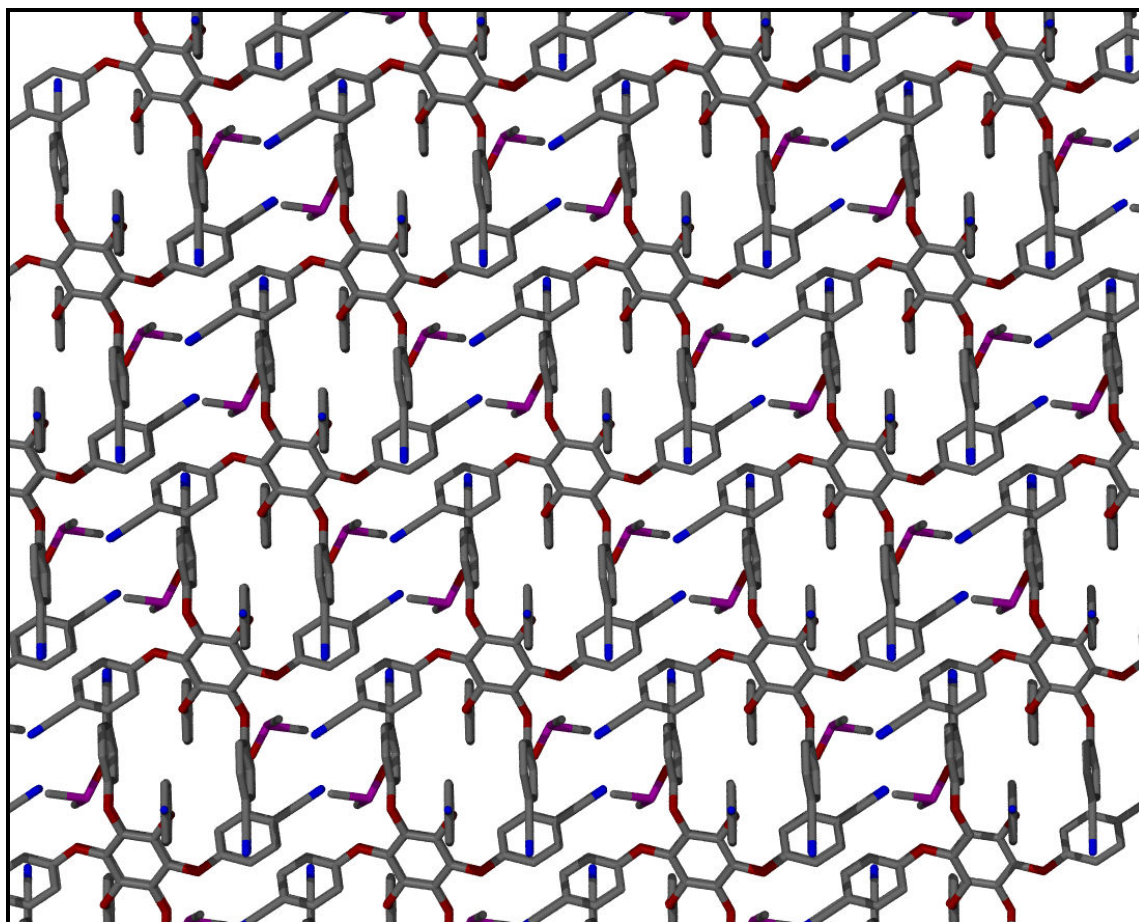


Figure S31. Packing diagram of **1f**, viewed along the *b* axis. Hydrogen atoms are omitted for clarity.

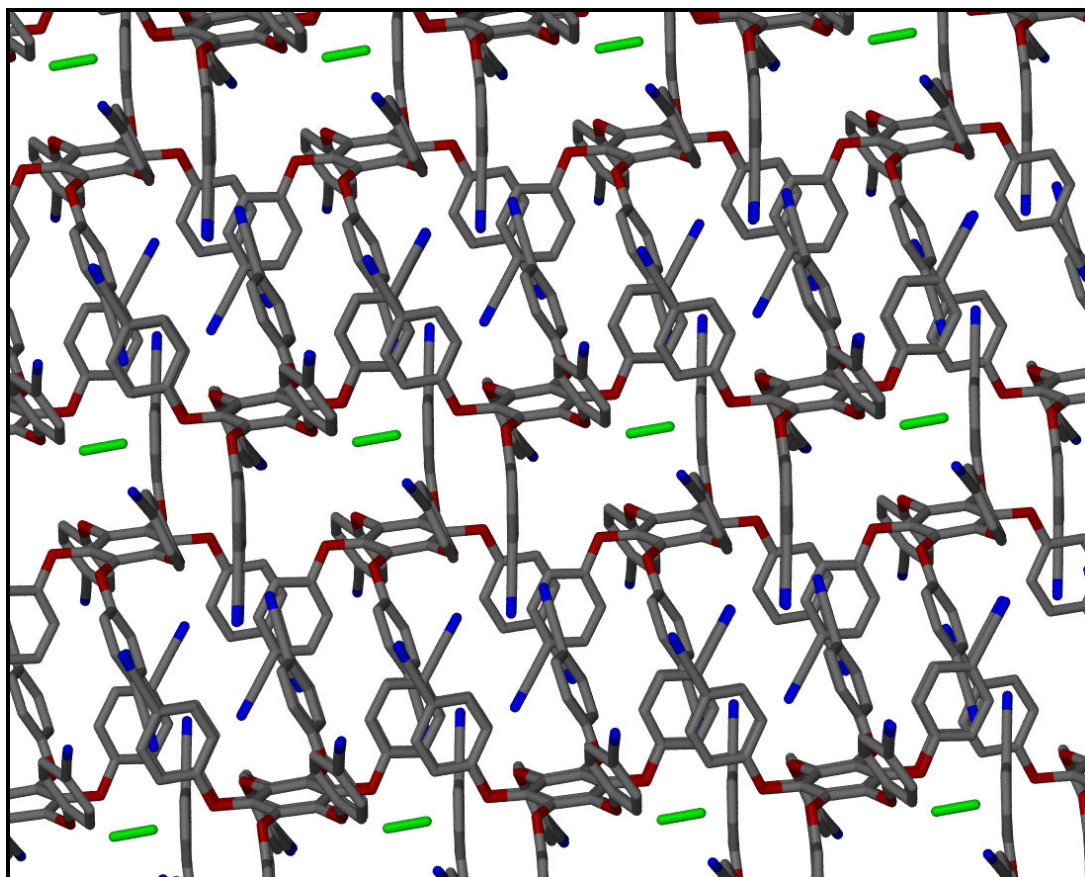


Figure S32. Packing diagram of **1g** viewed along the *c* axis. Hydrogen atoms are omitted for clarity. Methanol molecules are shown in green.

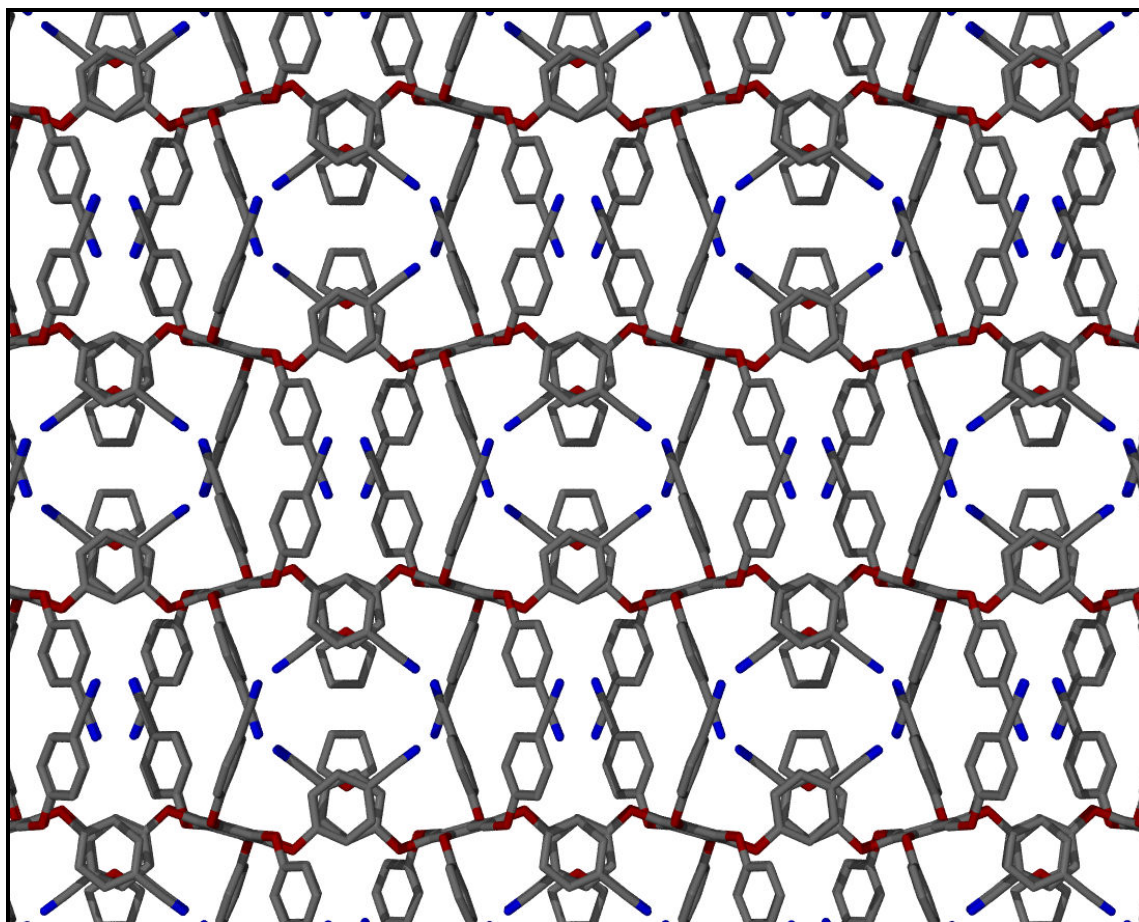


Figure S33. Packing diagram of **1h**, viewed along the *c* axis. Hydrogen atoms are omitted for clarity.

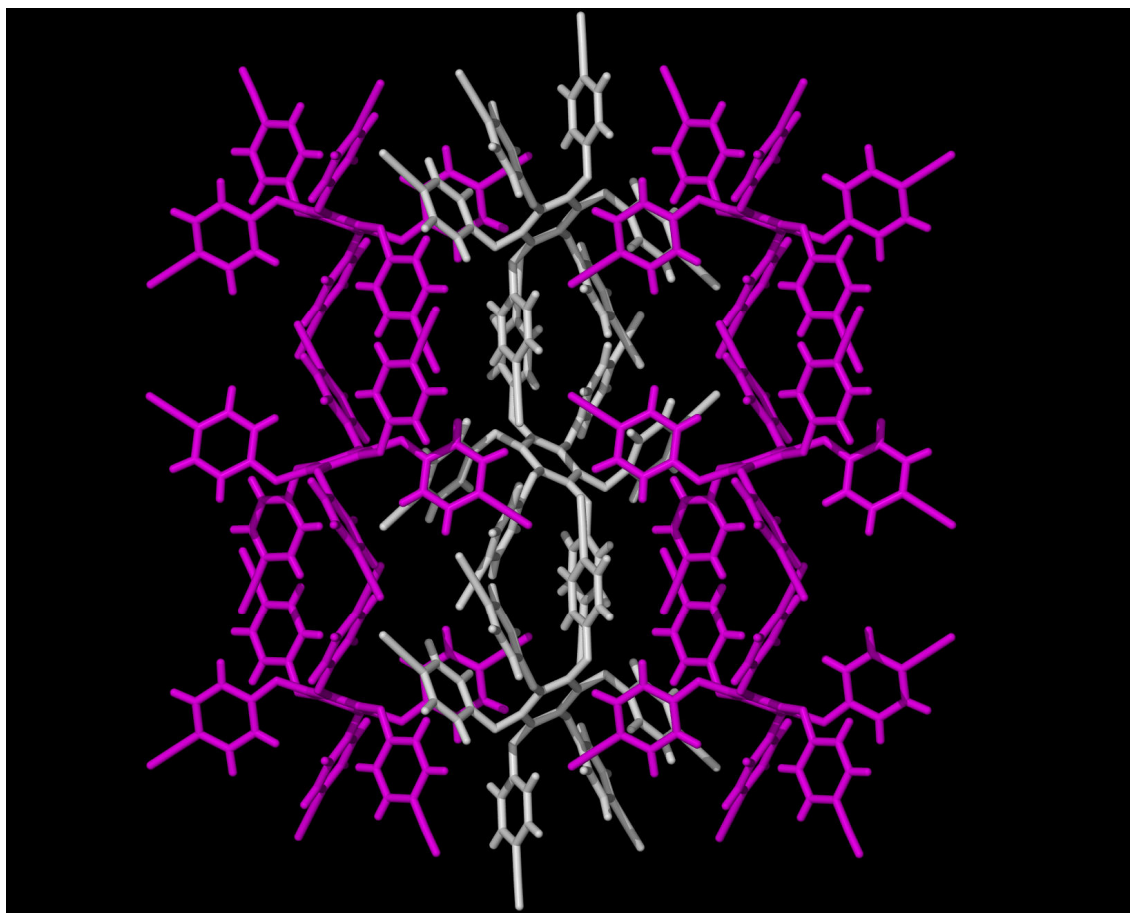


Figure S34. Packing diagram of **M1** viewed along [001]. This structure was obtained by melt-crystallization (described in ref 12 in the main text). Desolvation of all the solvates gives this crystal structures. The crystal structure contains two different conformations of molecule **1**. The purple molecules have the *ababab* conformation and the white molecules have the *aaabbb* conformation.