Supplementary Material (ESI) for New Journal of Chemistry

Supramolecular Networks of H-shaped Aromatic Phenol Host†

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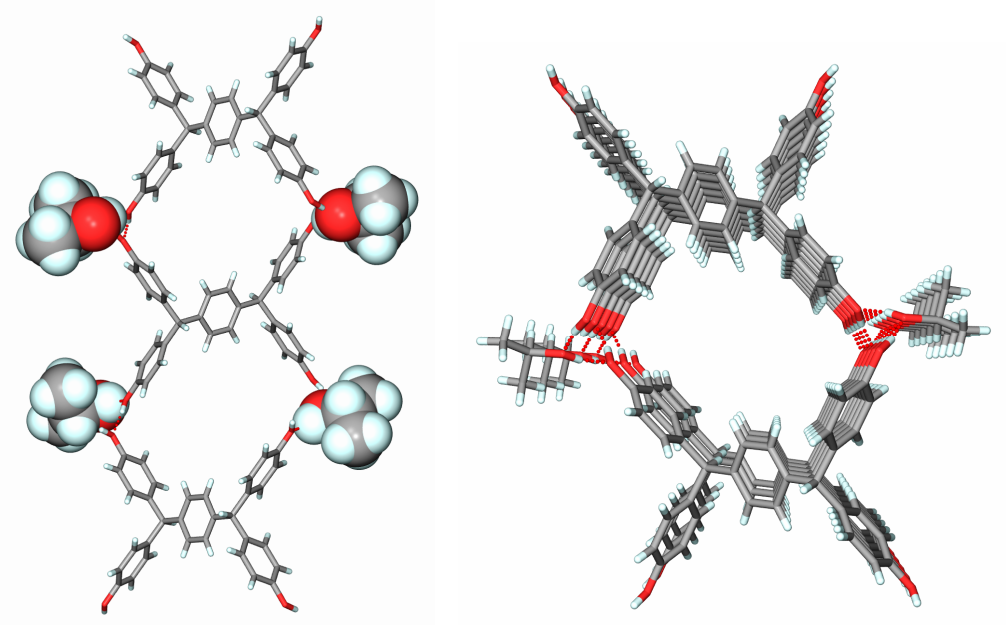
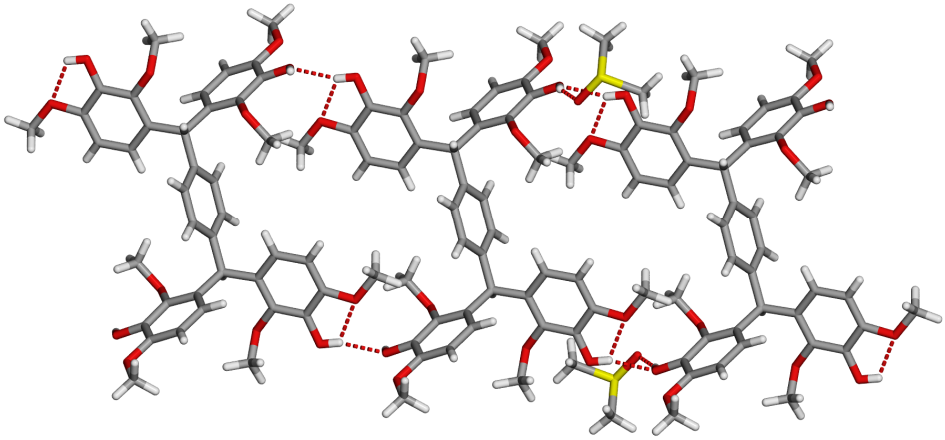
Electronic Supplementary Information (ESI)†

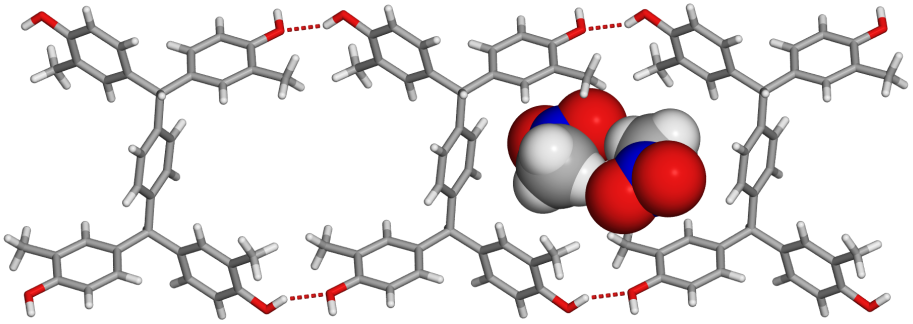


(a) (b)

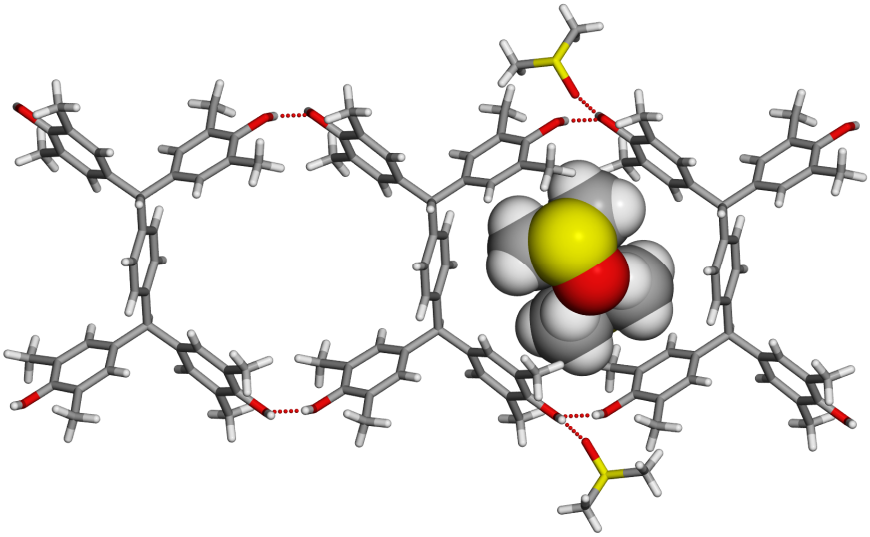
Fig. S1 (a) 1D ladder network along [001] in **1**•(i-PrOH)$_4$ in space group *C*2/*c* and (b) helical O–H···O trimer of host and guest molecules along [010]. Disordered solvent molecules between rung cavities (not shown) were Squeezed during structure refinement.



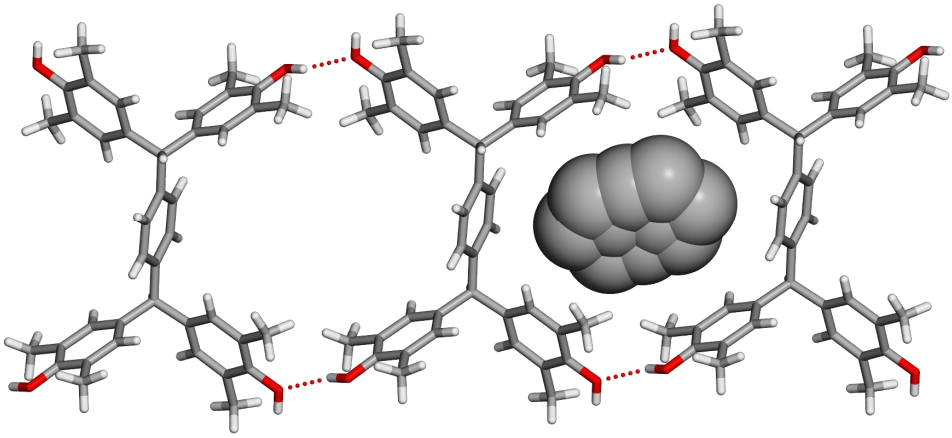
2•$(DMSO)_2$



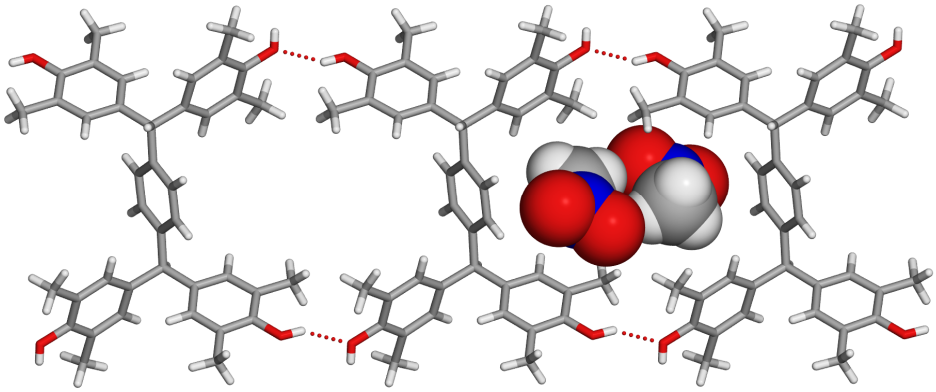
3•$(CH_3NO_2)_2$



4•$(DMSO)_2$



4•(Toluene)



4•$(CH_3NO_2)_2$

Fig. S2 1D ladder network and molecular positions of host and guest molecules. Solvent molecules reside in the ladder rung cavity except in **4**•$(DMSO)_2$ where methoxy groups are self-included.

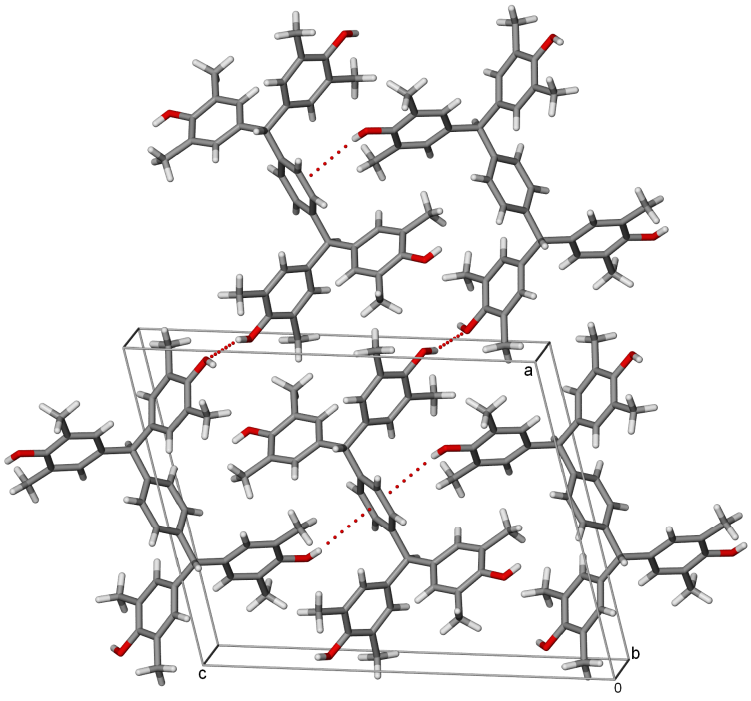


Fig. S3 Close packing of molecules in the crystal structure of guest-free **4**. There are no significant hydrogen bonds except a long O–H···O (2.41 Å, 158.8°) because of steric crowding by ortho-Me groups.

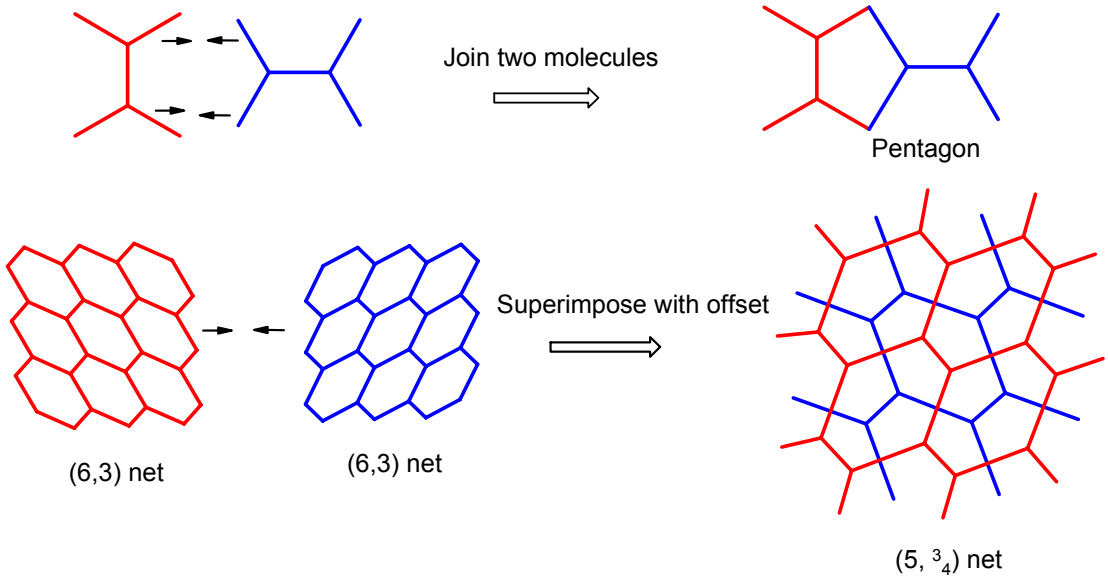


Fig. S4 The construction of a pentagon by the side-on approach of two H shaped tectons or the $(5,^{3}_{4})$ net by the offset superposition of two (6,3) hexagonal sheets.[12]

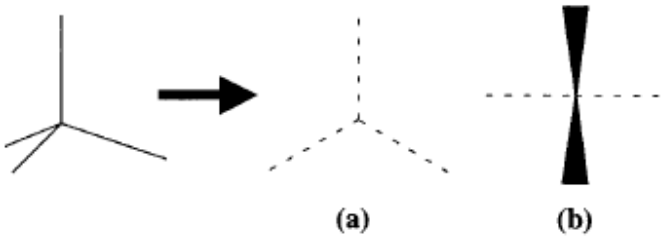
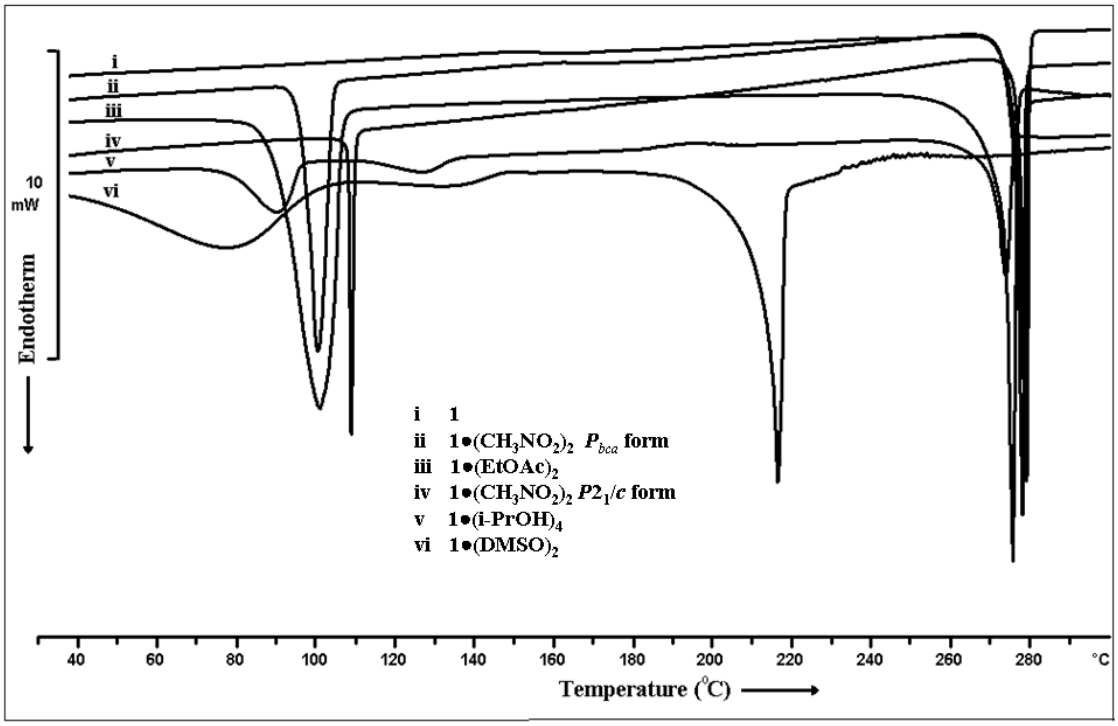
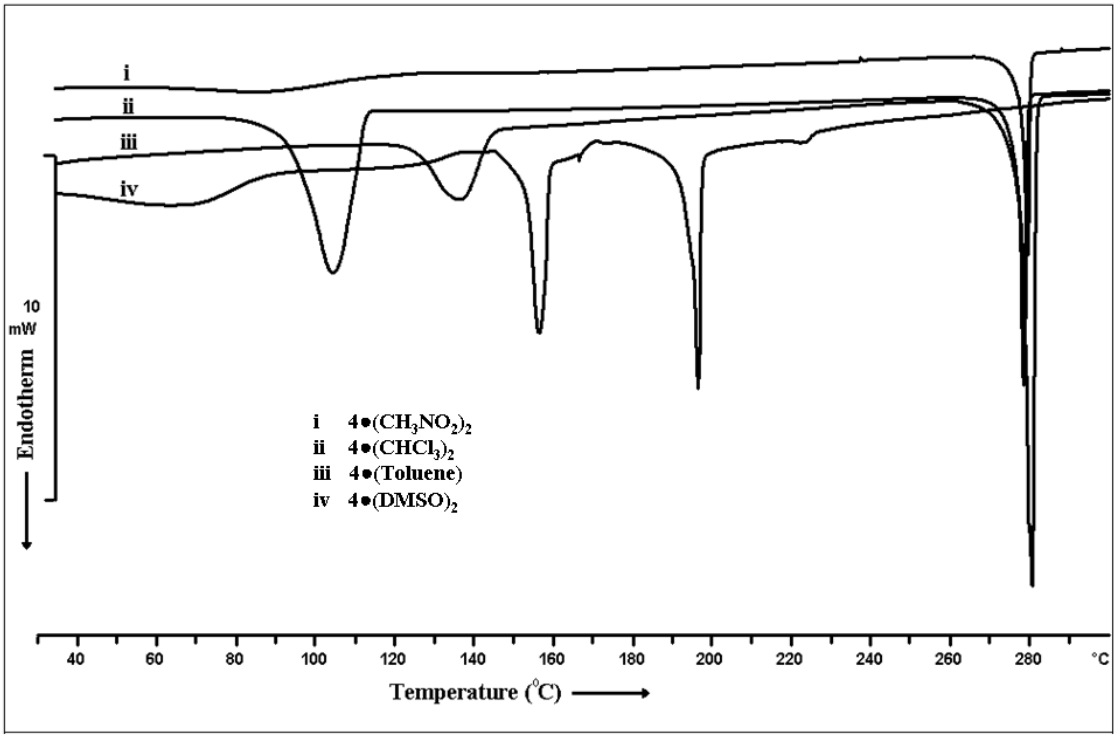


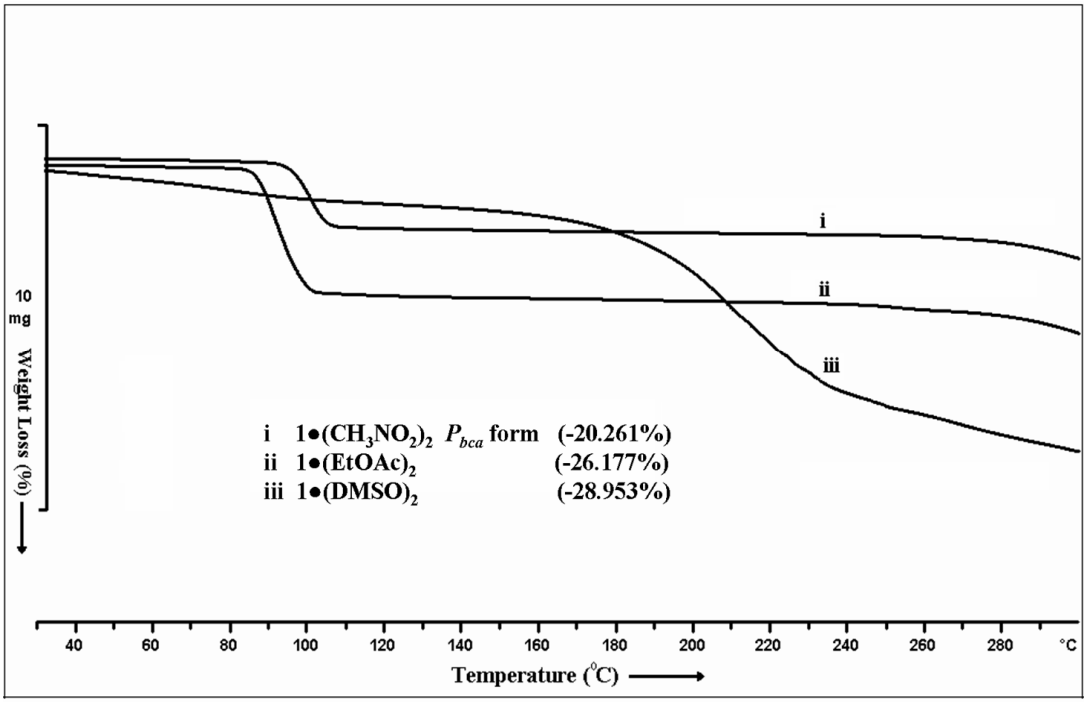
Fig. S5 Any tetrahedral node may behave as 3-connected (a) or 4-connected (b) node depending on the direction of viewing being a C_3 or C_2 axis.[21a]



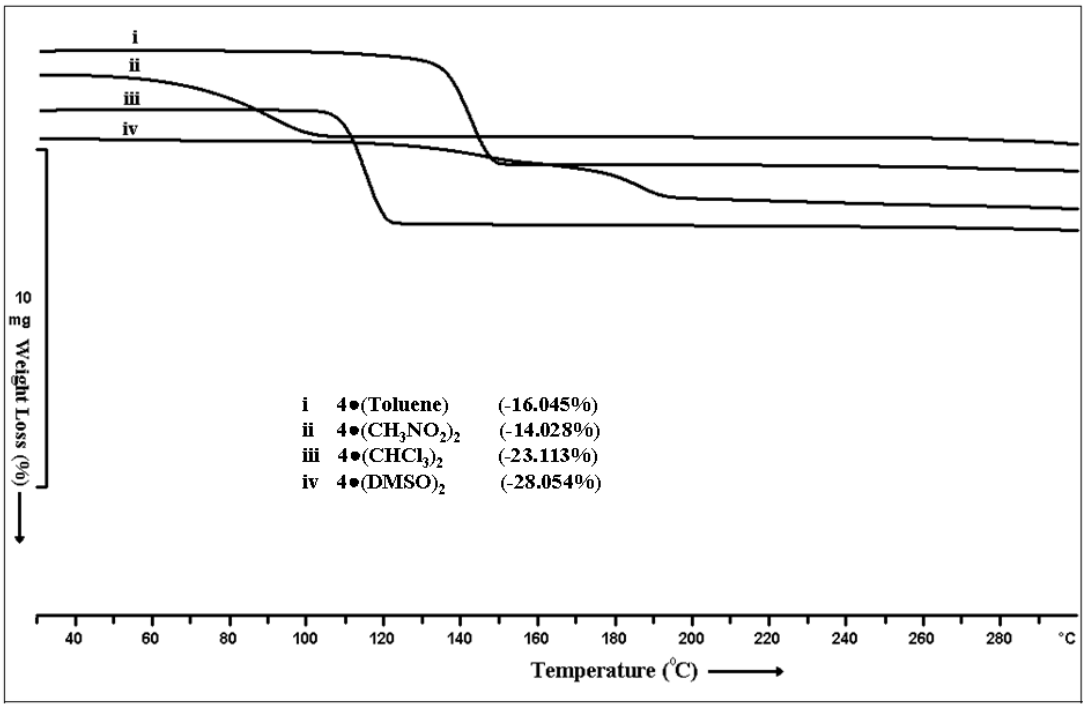
DSC of the **1** solvates



DSC of the **4** solvates



TGA of the **1** solvates



TGA of the **4** solvates

Fig. S6 DSC and TGA of **1** and **4** solvates. Endotherms and weight loss occur at the expected temperature. See Table 3 for thermal data.

Table S1 Distance of the molecular mean plane to phenolic O and tetrahedral C atoms (marked # in Fig. 1) in H-shaped structures (in Å).

Compound	Molecular mean plane···atom (Å)
1	0.87 (C23), 0.75 (O3), 0.64 (O4) 0.89 (C7), 0.66 (O1), 0.54 (O2)
1•$(DMSO)_2$	0.88 (C7), 0.59 (O1), 0.70 (O2)
1•$(EtOAc)_2$	0.90 (C7), 0.72 (O1), 0.65 (O2)
1•$(i\text{-}PrOH)_4$	0.84 (C7), 0.63 (O1), 0.66 (O2)
1•$(CH_3NO_2)_2$ *Pbca* form[12]	0.85 (C7), 0.60 (O1), 0.45 (O2)
1•$(CH_3NO_2)_2$ $P2_1/c$ form[12]	0.90 (C7), 0.68 (O1), 0.66 (O2)
1•$(4,4'\text{-}BipyNO)_2$	0.88 (C7), 0.62 (O1), 0.55 (O2), 0.84 (C20), 0.72 (O3), 0.45 (O4)
1•$(Phez)_{1.5}$	0.88 (C7), 0.53 (O1), 0.69 (O2) 0.89 (C23), 0.69 (O3), 0.60 (O4)
1•$(PyzNO)_2$	0.96 (C7), 0.69 (O1), 0.80 (O2)
1•$(Quinox)_2$	0.94 (C7), 0.60 (O1), 0.62 (O2)
1•$(CH_3OH)_2$ [5]	0.86 (C3), 0.49 (O1), 0.58 (O2)
1•$(C_2H_5OH)_2$ [5]	0.83 (C8), 0.46 (O1), 0.56 (O2)
1•$(CH_3CN)_2$ [5]	0.92 (C1), 0.63 (O1), 0.59 (O2) 0.87 (C18), 0.54 (O3), 0.54 (O4)
1•$(Dioxane)_2$ [5]	0.93 (C1), 0.62 (O1), 0.62 (O2) 0.87 (C20), 0.59 (O4), 0.57 (O5)
1•$(4,4'\text{-}Bipy)_2$ [5]	0.91 (C2), 0.78 (O1), 0.57 (O2)
2•$(Dioxane)_2$	0.46 (C7), 0.76 (O2), 0.86 (O5)
2•$(DMSO)_2$	0.65 (C7), 1.21 (O2), 0.94 (O5)
3•$(DMF)_2$	0.88 (C7), 0.29 (O1), 0.97 (O2)
3•$(CH_3NO_2)_2$	0.88 (C7), 1.12 (O1), 0.05 (O2)
4	0.88 (C7), 0.33 (O1), 0.74 (O2)
4•$(DMSO)_2$	0.83 (C7), 0.22 (O1), 0.78 (O2)
4•(Toluene)	0.84 (C7), 0.40 (O1), 0.90 (O2)
4•$(CH_3NO_2)_2$ [12]	0.91 (C7), 0.81 (O1), 0.40 (O2)
4•$(CHCl_3)_2$ [12]	0.79 (C7), 0.68 (O1), 0.48 (O2)
4•$(CH_3CN)_2$ [5]	0.83 (C1), 0.25 (O1), 0.55 (O2)