Supplementary Materials

for the manuscript “Methanol storage in high-pressure clathrate hydrates as a prolonged source of methane in large ocean worlds”
by Anna Pakhomova *et al.*

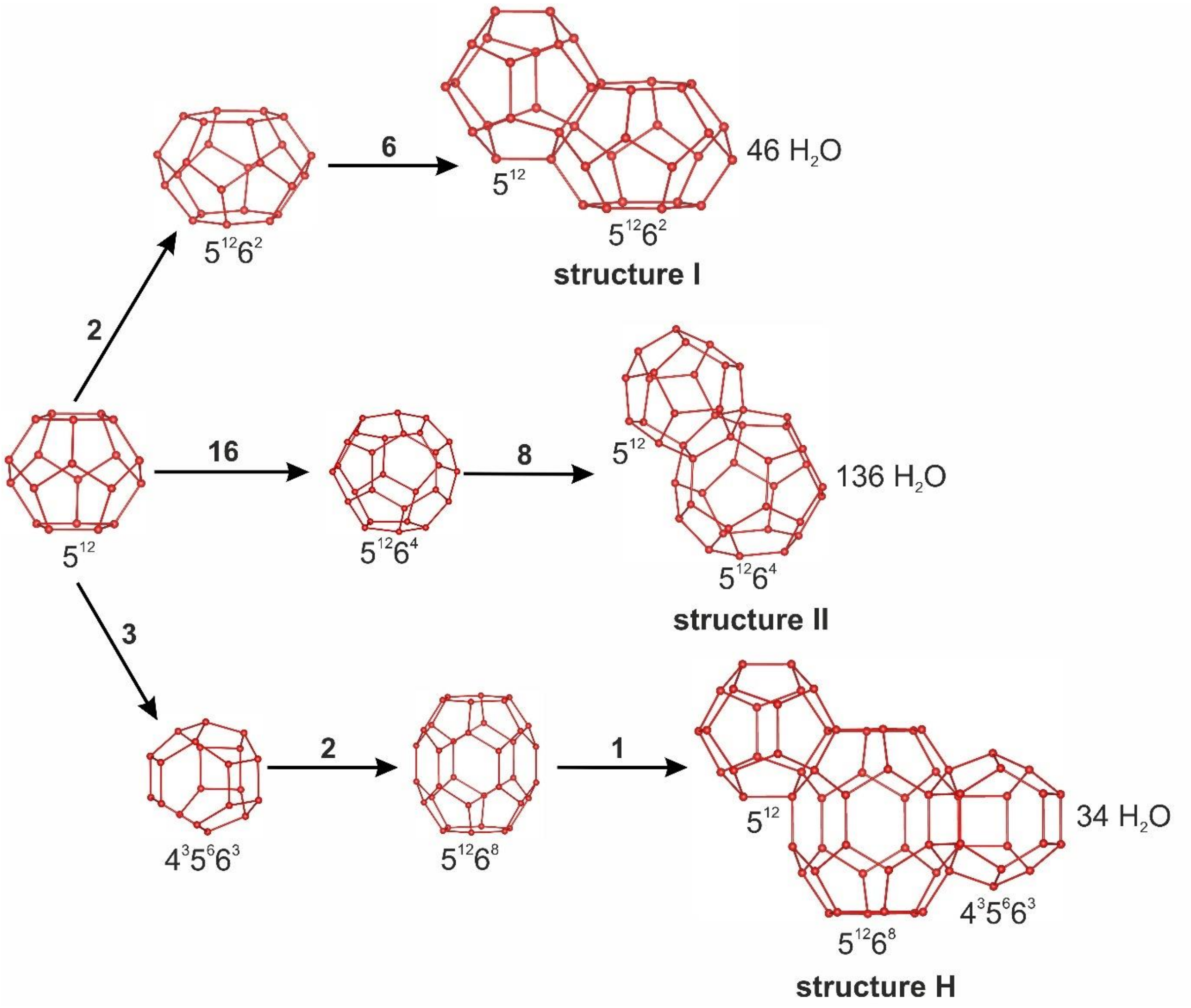


Figure S1. Framework topologies of sI, sII and sH clathrate hydrates that are formed under low temperature and near ambient pressure.

Text S1. Experimental Methods

S1.1 Temperature-pressure path of the THF-H_2O experiment (Experiment 1)

The followed P-T path in **Experiment 1** is given in Figure S2.

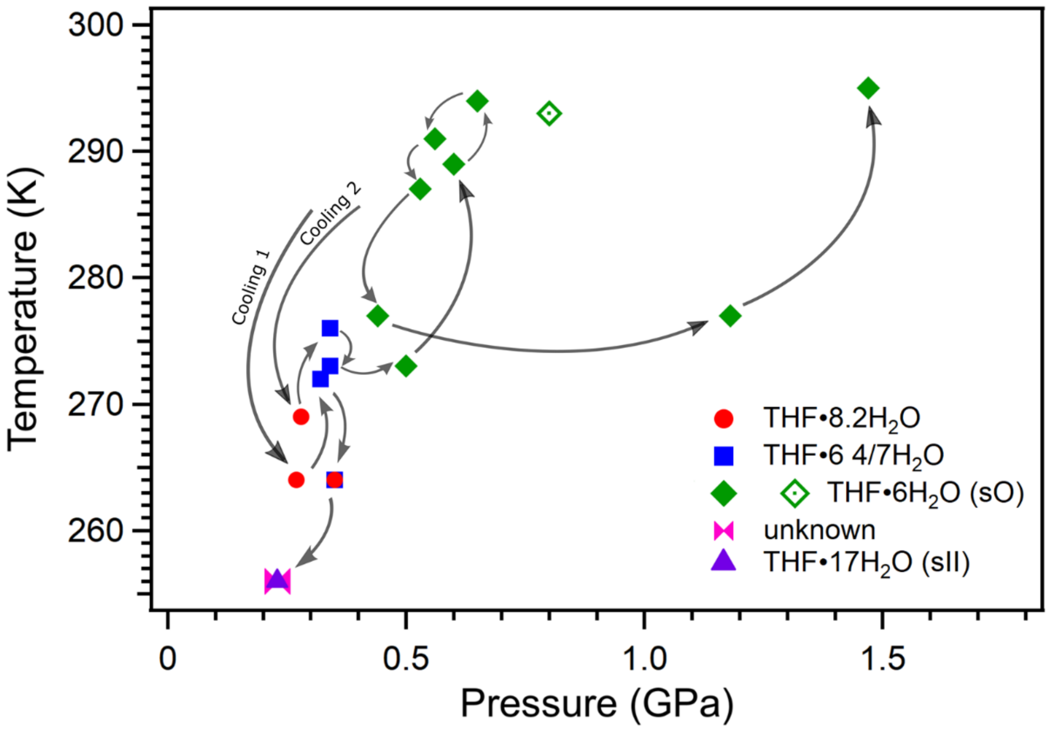


Figure S2. Pressure−temperature diagram indicating the conditions at which diffraction data for THF hydrates were collected in the present study in Experiment 1 (closed symbols). Open green rhombus corresponds to the P-T conditions where THF sO clathrate was previously observed by Kurnosov et al. (2004).

We started by cooling down the THF-H_2O (1:3) solution at 0.4 GPa. After crystallization of THF•8.2H_2O at 264 K (filled red circles in Figure S2, Figure S3a), the sample was slightly heated up in order to select few single crystals (Figure S3b). At 279 K the signs of melting have been observed and the sample was cooled down to 272 K. Upon cooling, the selected single crystal grew (Figure S3c). At this temperature and pressure of 0.32 GPa, THF•6 4/7H_2O hydrate was detected (filled blue squares in Figure S2). Upon further cooling to 264 K, the formation of THF•8.2H_2O has been observed again. At 264 K and 0.35 GPa THF•6 4/7H_2O and THF•8.2H_2O were found to be co-existing. During cooling, the crystals were continuously growing and filled almost all the chamber (Figure S3d,e). The sample was further cooled down and recrystallization occurred at 256 K (Figure S3f). The diffraction pattern of the polycrystalline sample which formed at these conditions was complex and represented a mixture of two phases: a sII clathrate hydrate (filled purple triangular in Figure S2) and an unknown phase with monoclinic symmetry and unit cell parameters *a* = 12.575(4) Å, *b*= 35.502(7) Å, *c* = 20.214(15) Å, β = 91.89(6)° (filled pink symbol in Figure S2). The quality of the data did not allow us to determine the crystal structure of the monoclinic phase. Upon heating, the sample melted at 274 K. Upon cooling, the solution crystallized again at 0.28 GPa and 269 K into THF•8.2H_2O (Figure S3g). The temperature was again slightly increased to select few single crystals (Figure S3h) and in order not melt the crystals, also the pressure was slightly increased. Upon pressurization, the crystals grew (Figure S3i). At 0.34 GPa and 276 K, the 6 4/7 hydrate was again detected. Further the sample was compressed to investigate the high-pressure region. Around 0.5 GPa, the 6 4/7 hydrate has recrystallized into THF•6H_2O (filled green rhombus in Figure S2) with polycrystalline texture. In order to select few single crystals, the temperature was increased to 294 K (Figure S3j). The THF•6H_2O was found to be stable up to the highest studied pressure of 1.47 GPa in the temperature range 277-295 K.

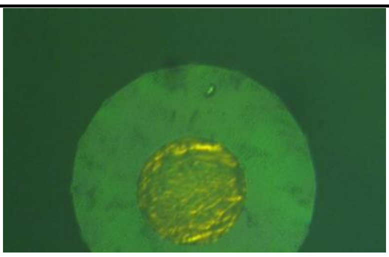
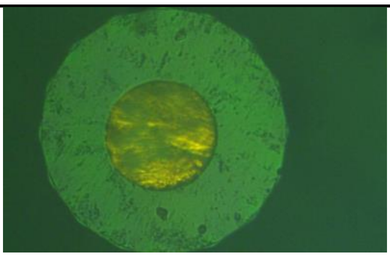
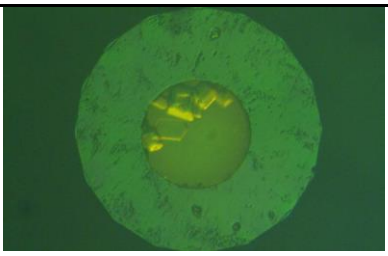
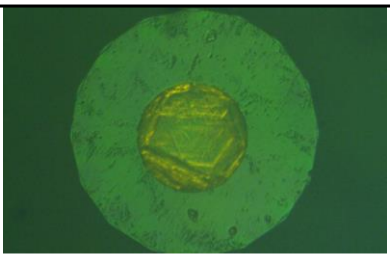
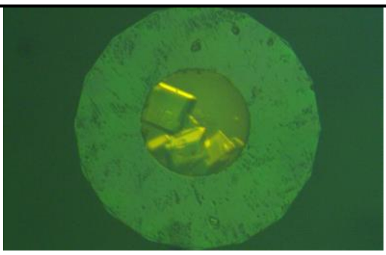
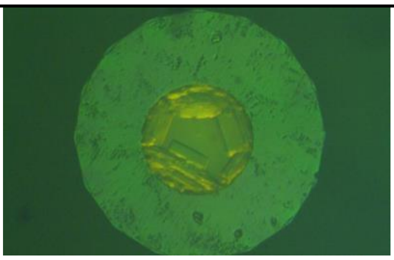
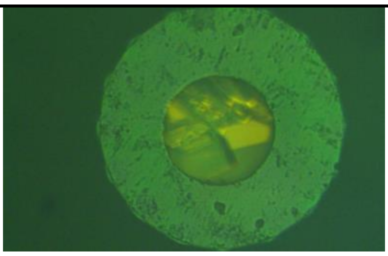
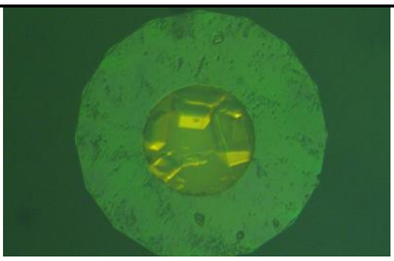
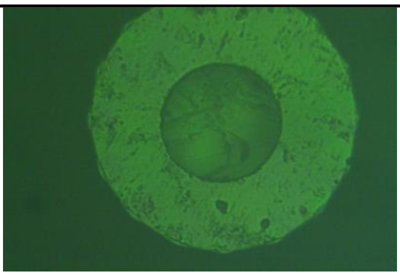
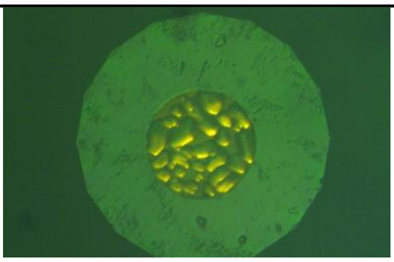
a		**THF•8.2H_2O** at 264 K and 0.27 GPa	**f**		**Mixture of sII and unknown phase** at 256 K and 0.23 GPa
b		**THF•6 4/7H_2O** Upon heating, ~ 279 K	**g**		**THF•8.2H_2O** at 269 K and 0.28 GPa
c		**THF•6 4/7H_2O** At 272 K and 0.32 GPa	**h**		Upon heating Between 269 and 276 K
d		**THF•8.2H_2O and THF•6 4/7H_2O** at 264 K and 0.35 GPa before cell centering	**i**		**THF•6 4/7 H_2O** at 273 K and 0.34 GPa
e		**THF•8.2H_2O** at 264 K and 0.35 GPa after cell centering	**j**		**THF•6H_2O** at 294 K and 0.65 GPa

Figure S3. Photos of the sample chamber with corresponding pressure-temperature conditions in the course of Experiment 1 (THF-H_2O solution). The diameter of the diamond culet is 600 μm.

S1.2 Temperature-pressure path of THF-MeOH-H_2O experiment (Experiment 2)

The followed P-T path in **Experiment 2** is given in Figure S4.

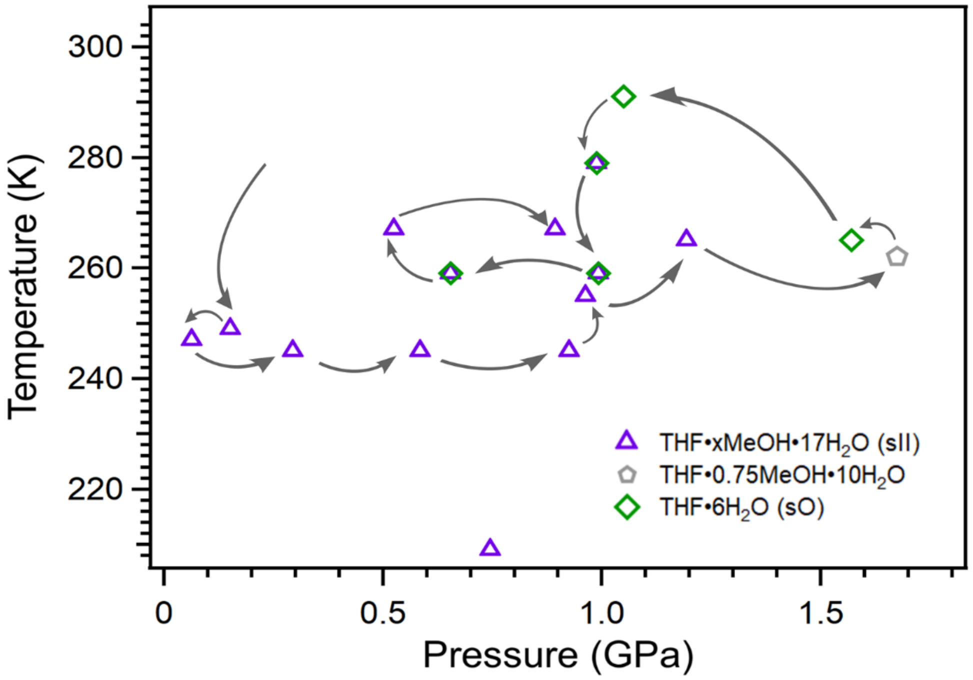
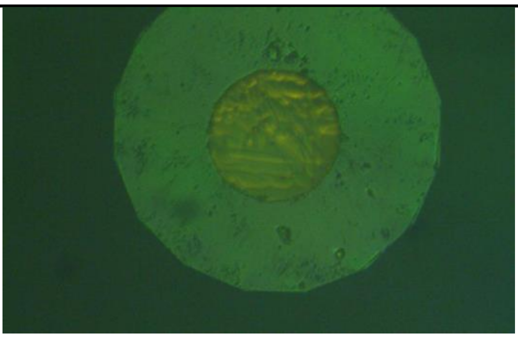


Figure S4. Pressure–temperature diagram indicating the conditions at which diffraction data for THF and THF-MeOH hydrates were collected in the present study in the Experiment 2.

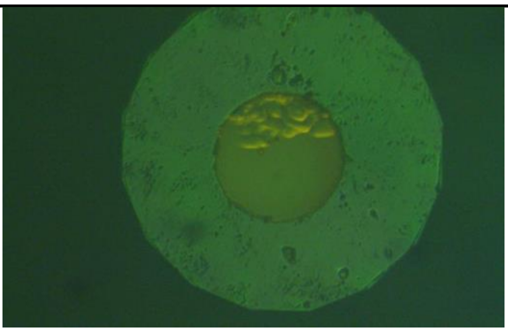
We started by cooling down the THF-methanol (MeOH)-H_2O solution, pressurised up to 0.35 GPa. The cubic sII clathrate crystallised at 249 K (open blue triangles in Figure S2, Figure S5a). The sample was heated up to 256 K to select few single crystals (Figure S5b) and then was cooled down to 247 K to preserve the selected crystals. Pressure was slightly increased to 0.3 GPa and temperature was decreased to 245 K to grow larger crystals (Figure S5c). At this temperature the sample was compressed up to 0.92 GPa. The sII phase was found to still be stable. In order to check the stability of this phase, it was heated to 255 K and further to 265 K. At 1.19 GPa and 265 K, only the sII was detected. Further pressure increase resulted in a formation of a new phase, determined as decahydrate (open grey pentagon in Figure S2). After the data collection at 1.67 GPa and 265 K, the sample has optically changed and the sample chamber became opaque (Figure S5d). This transformation resulted in the formation of a sO clathrate hydrate (open green rhombuses in Figure S2) causing a slight pressure drop to 1.57 GPa (Figure S5e). No optical changes have been observed upon heating up to 291 K and the sO clathrate was decompressed to 1.04 GPa (Figure S5f). Further the sample was cooled down and two phases have been detected at 279 K and 0.99 GPa: the sO and the sII. By decreasing the temperature from 279 to 259 K, the progressive growth of the sII phase was observed. At 259 K and 0.99 GPa still two phases were co-existing (Figure S5h). Pressure was decreased to 0.65 GPa where both phases still were present. The sample was warmed up to 267 K in order to destabilise one of the phases and indeed melting of the sO was observed upon temperature increase (Figure S5g). Pressure was increased up to 0.89 GPa where the sII was still present. The sII phase was preserved upon cooling down to 209 K (0.74 GPa).

a



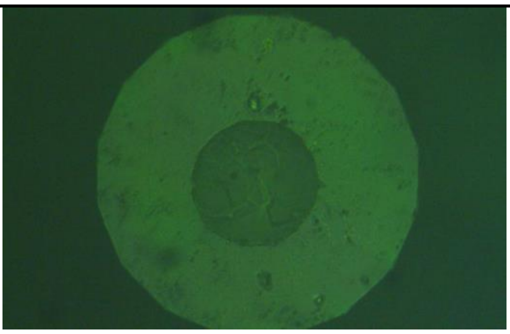
sII clathrate at 0.15 GPa and 249 K

b



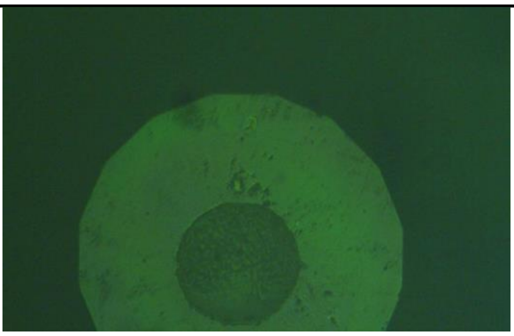
sII clathrate during crystal selection upon heating

c



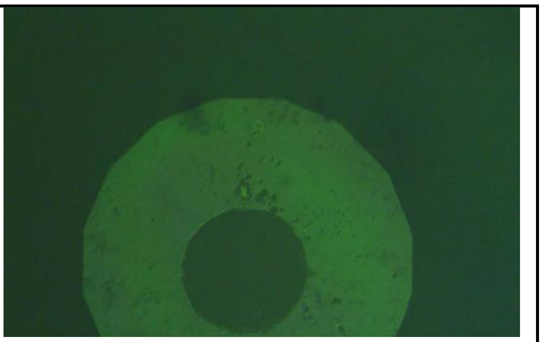
sII clathrate at 0.58 GPa and 245 K

d



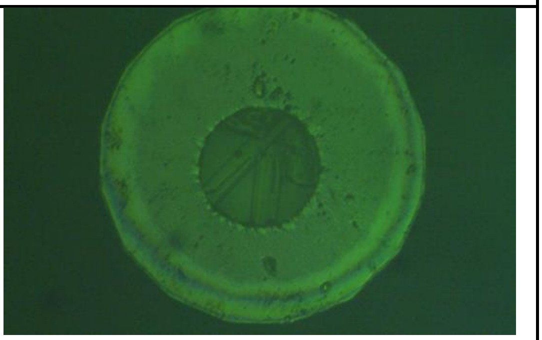
THF•0.75MeOH•10H_2O at 1.67 and 265 K

e



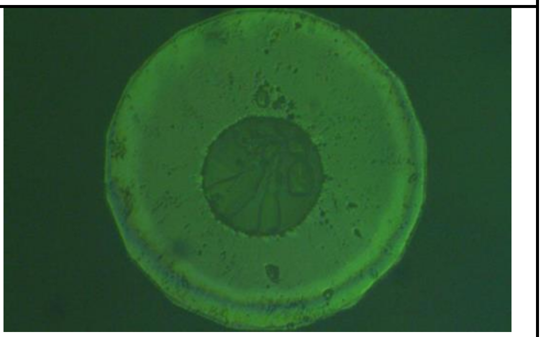
THF•6H_2O (sO) at 1.57 GPa and 265 K

f



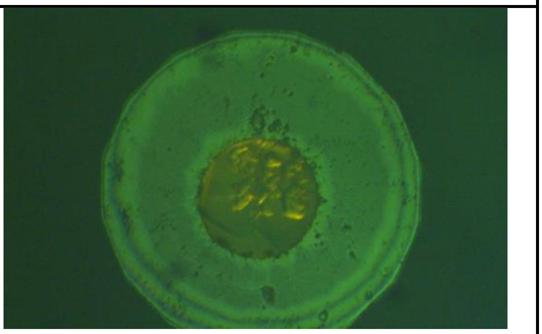
THF•6H_2O (sO) at 1.04 GPa and 291 K

g



THF•6H_2O (sO) at 0.99 GPa and 279 K

h



sII + THF•6H_2O (sO) at 0.99 GPa and 259 K

Figure S5. Photos of the sample chamber with corresponding pressure-temperature conditions in the course of Experiment 2 (THF-MeOH-H_2O solution). The diameter of the diamond culet is 600 μm.

Coordinates of the experimental points are summarized in Table S1:

Table S1. Experimental conditions of the observed phases in the Experiments **1** and **2**.

Experiment 1			Experiment 2		
P (GPa)	T(K)	Phase	P (GPa)	T(K)	Phase
0.27	264	THF•8.2H_2O	0.15	249	THF•*x*MeOH•17H_2O (sII)
0.32	272	THF•6 4/7H_2O	0.06	247	THF•*x*MeOH•17H_2O (sII)
0.35	264	THF•8.2H_2O + THF•6 4/7H_2O	0.29	245	THF•*x*MeOH•17H_2O (sII)
0.23	256	THF•17H_2O (sII) + unknown phase	0.58	245	THF•*x*MeOH•17H_2O (sII)
0.28	269	THF•8.2H_2O	0.92	245	THF•*x*MeOH•17H_2O (sII)
0.34	276	THF•6 4/7H_2O	1.19	265	THF•*x*MeOH•17H_2O (sII)
0.34	273	THF•6 4/7H_2O	1.67	265	THF• 0.75MeOH•10H_2O
0.50	273	THF•6H_2O (sO)	1.57	265	THF•6H_2O (sO)
0.60	289	THF•6H_2O (sO)	1.04	291	THF•6H_2O (sO)
0.65	294	THF•6H_2O (sO)	0.99	279	THF•6H_2O (sO) + sII
0.56	291	THF•6H_2O (sO)	0.99	259	THF•6H_2O (sO) + sII
0.53	287	THF•6H_2O (sO)	0.94	259	THF•6H_2O (sO) + sII
0.44	277	THF•6H_2O (sO)	0.65	259	THF•6H_2O (sO) + sII
1.18	277	THF•6H_2O (sO)	0.52	267	THF•*x*MeOH•17H_2O (sII)
1.47	295	THF•6H_2O (sO)	0.89	267	THF•*x*MeOH•17H_2O (sII)
			0.74	209	THF•*x*MeOH•17H_2O (sII)

Text S2. Structure solution and refinements

The crystal structures of several hydrates were solved using a dual-space algorithm implemented in the SHELXT program (Sheldrick 2015). The iterative structure refinements were performed with the use of the SHELXL program (Sheldrick 2015) built in the ShelXle (Hübschle et al. 2011) graphical user interfaces. Bragg reflections overlapping with reflections from the diamonds were excluded from the structure analysis. The details of structure refinements are given in the text below. The Crystallographic Information Files (CIFs) for the reported structures are deposited as Supporting Information.

Text S2.1. Structure refinement of THF·8.2H_2O

The intensity data of THF·8.2H_2O were collected at P = 0.27 GPa and T = 264 K (Figure S2a) in Experiment **1** (THF-H_2O solution). The THF·8.2H_2O hydrate is hexagonal, with unit-cell lattice parameters *a* = 12.3979(8) Å, *c* = 24.661(10) Å and space group $P6_3/mmc$. The direct solution produced a model with seven oxygen atoms (O1-O7) building the hydrogen-bonded framework, composed of four types of cages: two small cages $4^6 6^2$ (hexagonal prisms) and 5^{12} (pentagonal dodecahedra, D cage) and two large ones, $4^2 5^8 6^4{}_d$ (distorted, see below for the details) and $5^{12} 6^4$ (H cage). Regular geometry of these four cages is demonstrated in Figure S6 while comparison of the regular and distorted $4^2 5^8 6^4$ cages are given in Figure S7. As shown, due to the flattening of the buckled 5-membered faces, the two oxygens are separated by more than 5 Å thus "opening" the cage and forming the channels. The O1-O7 oxygens are fully occupied and their thermal displacement parameters were refined isotropically. At this step, R_1 was about 19% where R_1 is a standard measure of agreement between the crystallographic model (F_c) and the experimental X-ray diffraction data (F_o) and defined as $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$. Analysis of the remaining electron density maxima revealed the presence of another framework oxygen atom O8 featuring three-fold axial disorder. This results in the formation of unusual 7-membered distorted rings with O8-O4 separation of 2.672(15) Å. Other O-O distances, not including the O8, vary from 2.743(5) to 2.807(4) Å. The resulting framework topology is presented in the Figure 2a. Similar framework topology was reported previously for isopropylamine octahydrate, $10(CH_3)_2CHNH_2 \bullet 80H_2O$ (McMullan et al. 1970), but never for THF. Disordered THF molecules were detected in the large cages $4^2 5^8 6^4{}_d$ and $5^{12} 6^4$. In the cages $5^{12} 6^4$, two electron density maxima were assigned to two carbon atoms. Refinement of their site occupancy resulted close to unity within error, therefore the occupancy was constrained to 100%. Their thermal displacement parameters were refined anisotropically. This showed that the THF molecule is disordered in the *ab* plane around the [001] rotation axis (Figure S8). The disorder of THF in the larger $4^2 5^8 6^4$ cage is more severe. We defined the four carbon atoms that do not form any regular arrangement. Assuming the full occupancy of THF molecules, the stoichiometry of this hydrate is defined as $10THF \bullet 82H_2O$. The data quality did not allow us to refine hydrogen positions due to weak scattering of the compound at high 2θ angles and due to usage of a diamond anvil cell that limits access to the reciprocal space. This approach allowed us to refine the crystal structure to an R_1 of ~ 11 %.

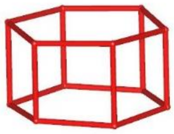
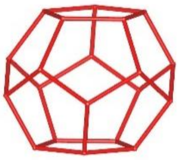
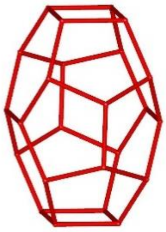
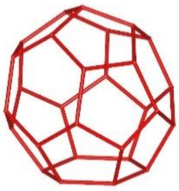
(a)	$\mathbf{4^{6}6^{2}}$ (hexagonal prisms) *vacant*	
(b)	$\mathbf{5^{12}}$ (pentagonal dodecahedra, D cage) *vacant*	
(c)	$\mathbf{4^{2}5^{8}6^{4}}$ *occupied*	
(d)	$\mathbf{5^{12}6^{4}}$ (H cage) *occupied*	

Figure S6. Regular geometry of cages $4^{6}6^{2}$ (hexagonal prisms), 5^{12} (pentagonal dodecahedra, D cage), $4^{2}5^{8}6^{4}$, and $5^{12}6^{4}$ (H cage) composing the hydrogen-bonded framework of THF·8.2H_2O.

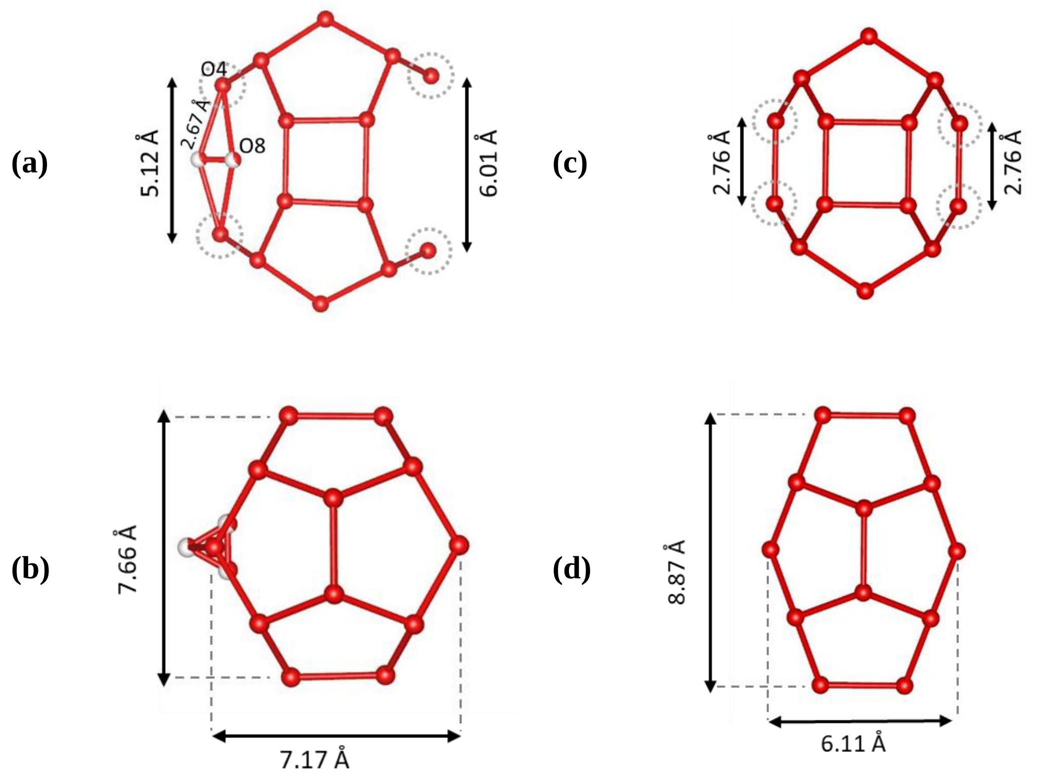
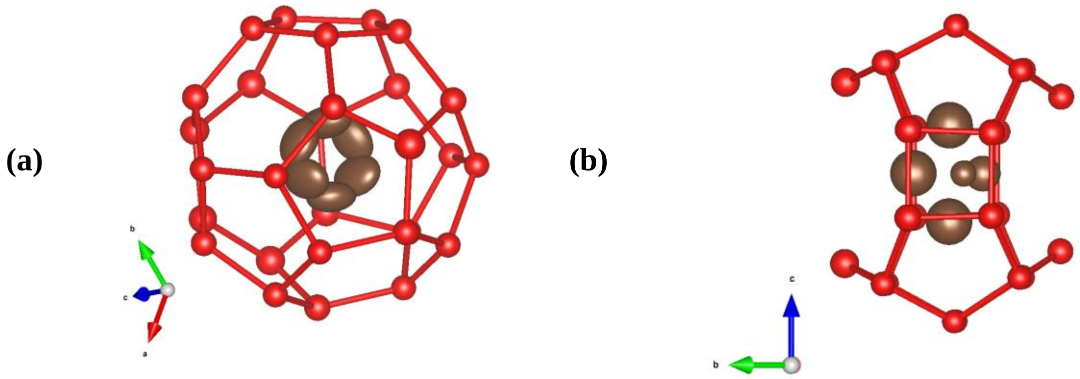


Figure S7. Comparison of the regular (right) and distorted (left) geometry of $4^2 5^8 6^4$ cages along different projections. The regular polyhedron is drawn using the data on sT acetone clathrate from Pakhomova et al. 2022. Red circles represent oxygens of hydrogen-bonded water molecules.



$5^{12}6^4$ $4^25^86^4{}_d$

Figure S8. Disordered THF molecules in the $5^{12}6^4$ (a) and $4^25^86^4{}_d$ (b) cages of THF·8.2H_2O. Ellipsoids are drawn at 50% probability level. Red balls represent oxygens of hydrogen-bonded water molecules while brown balls and ellipsoids represent parts of the disordered THF molecules.

Text S2.2. Structure refinement of THF•6 4/7H_2O

The intensity data of THF•6 4/7H_2O were collected on a selected crystal at P = 0.32 GPa and T = 272 K (Figure S3c) in Experiment **1**. THF•6 4/7H_2O is hexagonal, with space group *P*6/*mmm* and unit cell dimensions a = 12.3899(12) and c = 14.7002(18) Å. The direct solution produced a model with R_1~30 % and with five oxygen atoms (O1-O5) building the hydrogen-bonded framework. Refinement of site occupancies of O1-O4 atoms resulted in close to unity within error, therefore their occupancy was constrained to 100%. Their thermal displacement parameters were refined isotropically. The O5 atom revealed high thermal displacement parameter and therefore was refined anisotropically. Defined in this way the hydrogen-bonded framework is composed of four types of cages (Figure S9): $4^6 6^2$ (hexagonal prisms), $5^{12}6^2{}_d$, $4^2 5^8 6^4{}_d$, $5^{12}6^3{}_d$ where the former three are distorted due to the O5-O5 separation of ~3.5 Å (Figure S10). Other distances between adjacent oxygens of the host framework vary in the range 2.743(7)-2.845(10) Å. The resulting framework topology is presented in the Figure 2b. Analysis of the remaining electron density maxima revealed the presence of highly disordered THF molecules in the cages $5^{12}6^2{}_d$, $4^2 5^8 6^4{}_d$, $5^{12}6^3{}_d$. The highest electron density maxima above ~0.3 e/$Å^3$ were assigned to carbon atoms and their occupancy and thermal anisotropic parameters have been refined (Figure S11). The data quality did not allow us to refine hydrogen positions due to the weak scattering of the compound at high 2θ angles and due to the diamond anvil cell that limits access to the reciprocal space. This approach allowed us to refine the crystal structure to R_1 of ~ 12 %.

The same framework topology was recently described for 6 3/7 cyclobutylamine (cBA) hydrate (Dobrzycki et al. 2016) but never for THF. Dobrzycki et al. (2016) reported a partial substitution of the O5 framework oxygen with the amino group of the cBA occupying the $5^{12}6^2$ cages. In our case, we do not see such effect and define the stoichiometry of this hydrate as 7THF•46H_2O (THF•6 4/7 H_2O).

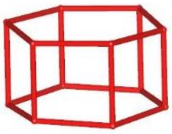
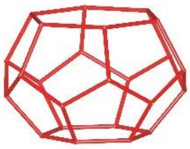
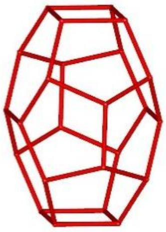
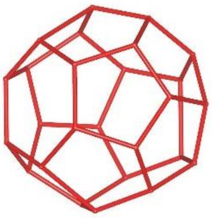
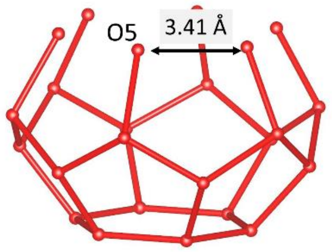
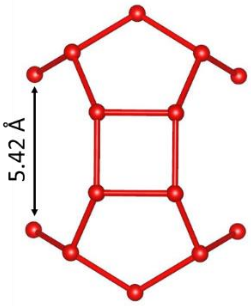
(a)	$4^6 6^2$ (hexagonal prisms) *vacant*	
(b)	$5^{12} 6^2$ *occupied*	
(c)	$4^2 5^8 6^4$ *occupied*	
(d)	$5^{12} 6^3$ *occupied*	

Figure S9. Regular geometry of cages $4^6 6^2$ (hexagonal prisms), $5^{12} 6^2$, $4^2 5^8 6^4$ and $5^{12} 6^3$ composing the hydrogen-bonded framework of THF 6 4/7 hydrate.

(a) $5^{12}6^{2}$



(b) $4^{2}5^{8}6^{4}$



(c) $5^{12}6^{3}$

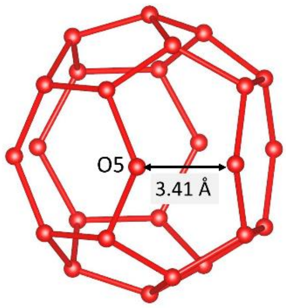
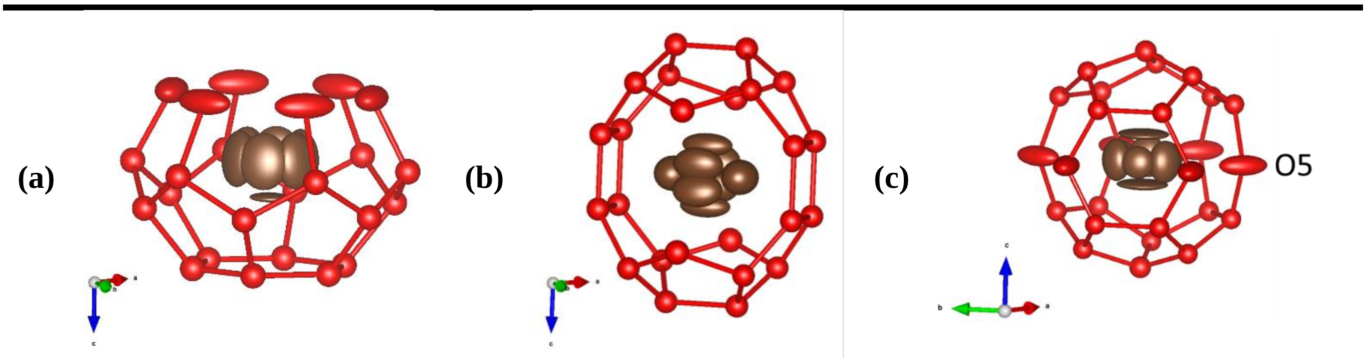


Figure S10. Distorted geometry of $5^{12}6^{2}$ (a), $4^{2}5^{8}6^{4}$ (b) and $5^{12}6^{3}$ (c) cages composing the hydrogen-bonded framework of THF 6 4/7 hydrate. Red balls represent oxygens of hydrogen-bonded water molecules.



$5^{12}6^{2}_{d}$ | **$4^{2}5^{8}6^{4}_{d}$** | **$5^{12}6^{3}_{d}$**

Figure S11. Disordered THF molecules in the $5^{12}6^{2}_{d}$, $4^{2}5^{8}6^{4}_{d}$ and $5^{12}6^{4}$ cages of THF 6 4/7 H_2O hydrate. Ellipsoids are drawn at 50% probability level. Red balls represent oxygens of hydrogen-bonded water molecules while brown balls and ellipsoids represent parts of the disordered THF molecules.

Text S2.3. Structure refinement of THF•6H_2O (sO)

The intensity data were collected on a selected crystal at P = 1.05 GPa and T = 282 K in Experiment **1**. THF•6H_2O (sO) is orthorhombic, with space group $P2_12_12_1$ and unit cell dimensions a = 12.6149(10), b = 11.5016(6), and c = 6.6353(2) Å. The direct solution produced a model with R_1~13 % with three oxygen atoms (O1-O3) building the hydrogen-bonded framework and three carbon atoms located in its voids resembling geometry of a THF molecule. One of the intraframework carbon atoms was later assigned to the oxygen of THF molecule. All thermal displacement parameters were refined anisotropically. The THF molecule does not reveal high disorder however the APDs of its atoms are larger compared to the framework oxygens. The distances between adjacent oxygens of the host framework vary in the 2.762(5)−2.848(5) Å range. In contrast to the low-pressure clathrates of this study, the sO framework is constructed from unique cage type $4^45^46^6$ (Figures S12, Figure 2d). The data quality did not allow us to refine the hydrogen positions due to the weak scattering of the compound at high 2θ angles and due to the diamond anvil cell that limits access to the reciprocal space. The crystal structure was refined to 9.5 %.

The sO structure was previously described for THF (Kurnosov et al. 2004) at 0.8 GPa and acetone (Manakov et al. 2007; Pakhomova et al. 2022) clathrate hexahydrates. Interestingly, our refinement shows that the oxygen of the THF molecule is located at 3.493(9) Å from the closest framework oxygen, indicating that there is no host-guest hydrogen bonding, as it was previously described for the acetone clathrate of the same structure type (Pakhomova et al. 2022).

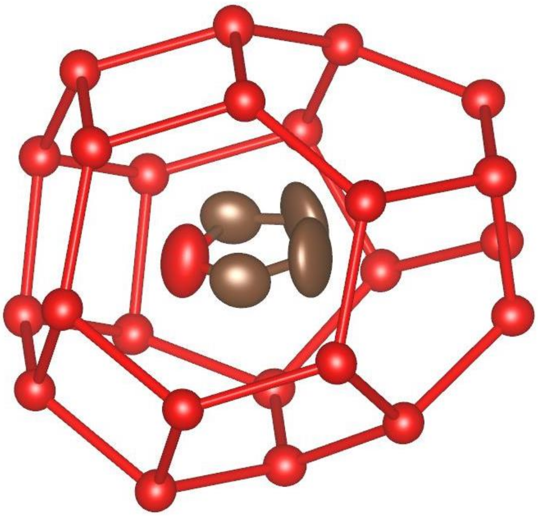


Figure S12. The $4^4 5^4 6^6$ cage composing the framework of the sO THF clathrate hydrate. The ellipsoids are drawn at 50% probability level. Red balls represent oxygens of hydrogen-bonded water molecules. Red and brown ellipsoids represent oxygen and carbons atoms of THF molecule, respectively.

Text S2.4. Structure refinement of THF•*x*MeOH•17H_2O (sII)

The data presented here were collected in the course of Experiment 2 (THF-MeOH-H_2O solution). Upon cooling of the pressurised solution, the cubic sII clathrate, with space group *Fd*-3*m* and unit cell dimension *a* = 12.644(4) Å has crystallised at 0.15 GPa and 249 K. The direct solution produced a model with three oxygen atoms (O1-O3) building the hydrogen-bonded framework. The defined hydrogen-bonded framework is composed of two types of cages: small 5^{12} cages (D) and large $5^{12}6^4$ (H) (Figure S1, S13). Analysis of the remaining electron density maxima revealed the presence of a 1.5 e/Å^3 electron density peak in the center of the 5^{12} cages that was assigned to the carbon atom (C1) of the methanol molecule. Several peaks in the $5^{12}6^4$ cage were assigned to carbon atoms of the highly disordered THF molecules. The remaining electron density peak in the proximity of the C1 was defined as an oxygen atom of the methanol molecule (O4). Upon pressurisation at nearly the same temperature of 245-249 K, the sII clathrate persisted at least up to 0.92 GPa. At every pressure point, occupancy and anisotropic displacement parameters of the O1-O3 atoms were refined. The occupancy of C1 was refined as well while its thermal parameter was fixed to the value refined at the highest pressure studied when its occupancy reaches unity. The evolution of the unit-cell parameters, refined occupancies, and selected distances versus pressure are given in Table S2 and S3. We note that C1 is located at a special position resulting in a larger error in the determination of the site occupancy as described in de Wolff (1966). The data quality did not allow us to refine the hydrogen positions due to the weak scattering of the compound at high 2θ angles and due to the diamond anvil cell that limits access to the reciprocal space. This approach allowed us to refine the crystal structure to R_1 of 7-8 % at all pressure points.

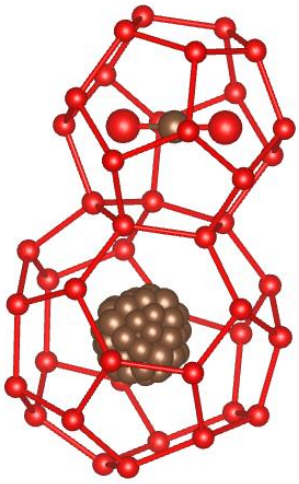


Figure S13. Two cages building the framework of sII THF-MeOH clathrate hydrate. Red and brown balls represent oxygen and carbon atoms, respectively.

Table S2. Evolution of unit cell parameters and occupancies of selected atomic sites of sII THF-MeOH clathrate hydrate upon pressurization at about 245-249 K.

dataset	**P (GPa)**	**T (K)**	**a (Å)**	**V(Å^3)**	**C1**	**O4**	**O1**	**O2**	**O3**
_0008	0.152	249	17.2978(6)	5175.7(5)	0.62(9)	0.05(2)	1.01(13)	0.93(12)	0.82(11)
_0016	0.2945	247	17.2292(4)	5114.4(4)	0.69(10)	0.08(4)	1.01(15)	1.01(15)	0.88(13)
_0021	0.585	245	17.0543(4)	4960.2(3)	1	0.034(17)	0.99(5)	0.89(5)	0.85(6)
_0023	0.926	245	16.8867(5)	4815.4(4)	1	-	0.94(8)	0.88(7)	0.88(9)

Table S3. Evolution of selected bond distances of sII THF-MeOH clathrate upon pressurization at about 245-249 K.

dataset	**P (GPa)**	**T (K)**	**C1-O1 (Å)**	**C1-O2 (Å)**	**C1-O3 (Å)**
_0008	0.152	249	3.9583(10)	3.8489(12)	3.74509(12)
_0016	0.2945	247	3.9444(9)	3.8390(11)	3.73023(8)
_0021	0.585	245	3.9046(11)	3.7940(13)	3.69236(8)
_0023	0.926	245	3.8666(16)	3.7562(19)	3.65607(10)

Text S2.4. Structure refinement of THF•0.75MeOH•10H_2O (decahydrate)

The intensity data of THF•0.75MeOH•10H_2O decahydrate were collected on a selected crystal at P = 1.67 GPa and T = 265 K in Experiment 2. THF•10H_2O is hexagonal, with space group *P*6/*mmm* and unit cell dimensions *a* = 11.8229(9), and *c* = 11.949(4) Å. The direct solution produced a model with R_1~30% and with five oxygen atoms (O1-O5) building the hydrogen-bonded framework. Refinement of the site occupancies of oxygen atoms resulted in close to unity within error, therefore their occupancy was constrained to 100%. Thermal displacement parameters of the O1-O4 atoms were refined isotropically. The O5 atom revealed high thermal displacement parameter and therefore was refined anisotropically. Defined in this way the hydrogen-bonded framework is composed of three types of cages (Figure S14): 5^{12}, $5^{12}6^2{}_d$, $5^{12}6^3{}_d$, where the former two are slightly distorted due to the O5-O5 separation of ~3 Å. Analysis of the remaining electron density maxima revealed the presence of disordered THF molecules in the cages $5^{12}6^2{}_d$ and $5^{12}6^3{}_d$. The highest electron density maxima above ~0.3 e/Å^3 in the $5^{12}6^2{}_d$ and $5^{12}6^3{}_d$ cages were assigned to carbon atoms and both their occupancy and thermal anisotropic parameters have been refined (Figure S15a,b). The strong electron density peak in the center of the 5^{12} cage was assigned to the carbon atom of the methanol molecule (Figure S15c). The data quality did not allow us to refine the hydrogen positions due to the weak scattering of the compound at high 2θ angles and due to the diamond anvil cell that limits access to the reciprocal space. This approach allowed us to refine the crystal structure to R_1 of ~ 12 %.

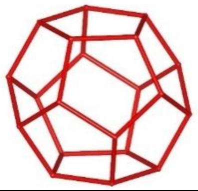
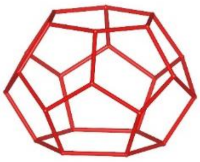
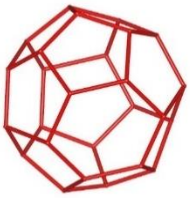
(a)	5^{12} D *occupied*	
(b)	$5^{12}6^2$ *occupied*	
(c)	$5^{12}6^3$ *occupied*	

Figure S14. Regular 5^{12}, $5^{12}6^2$, $5^{12}6^3$ case composing THF-MeOH decahydrate.

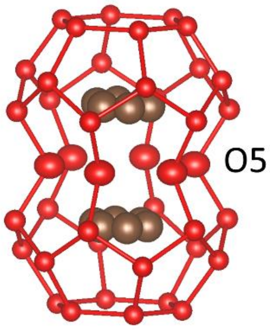
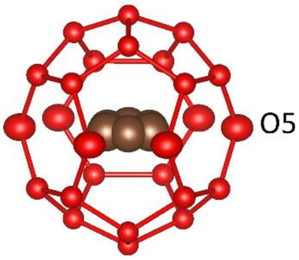
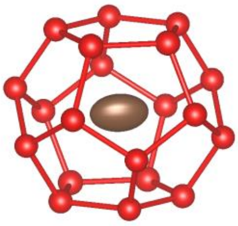
(a)		stack of $5^{12}6^2_d$ cages along the *c* axis
(b)		$5^{12}6^3_d$
(c)		5^{12} cage occupied by MeOH molecule

Figure S15. Occupancy of the 5^{12}, $5^{12}6^2_d$, and $5^{12}6^3_d$ cases composing THF-MeOH decahydrate. The ellipsoids are drawn at 50% probability level.

References

de Wolff, P.M. (1966) A simple rule for the electron-density error at special positions. Acta Crystallographica, 20, 141–141.

Dobrzycki, Ł., Pruszkowska, K., Boese, R., and Cyrański, M.K. (2016) Hydrates of Cyclobutylamine: Modifications of Gas Clathrate Types sI and sH. Crystal Growth & Design, 16, 2717–2725.

Hübschle, C.B., Sheldrick, G.M., and Dittrich, B. (2011) ShelXle: a Qt graphical user interface for SHELXL. Journal of Applied Crystallography, 44, 1281–1284.

Kurnosov, A.V., Komarov, V.Y., Voronin, V.I., Teplykh, A.E., and Manakov, A.Y. (2004) New Clathrate Hydrate Structure: High-Pressure Tetrahydrofuran Hydrate with One Type of Cavity. Angewandte Chemie International Edition, 43, 2922–2924.

Manakov, A.Yu., Ogienko, A.G., Komarov, V.Yu., Ancharov, A.I., and Sheromov, M.A. (2007) High-pressure clathrate hydrate of acetone. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 58, 317–320.

McMullan, R.K., Jeffrey, G.A., and Panke, D. (1970) Polyhedral Clathrate Hydrates. XVI. Structure of Isopropylamine Octahydrate. The Journal of Chemical Physics, 53, 3568–3577.

Pakhomova, A., Collings, I.E., Journaux, B., Petitgirard, S., Boffa Ballaran, T., Huang, D., Ott, J., Kurnosov, A., Hanfland, M., Garbarino, G., and others (2022) Host–Guest Hydrogen Bonding in High-Pressure Acetone Clathrate Hydrates: In Situ Single-Crystal X-ray Diffraction Study. The Journal of Physical Chemistry Letters, 13, 1833–1838.

Sheldrick, G.M. (2015) Crystal structure refinement with SHELXL. Acta Crystallographica Section C: Structural Chemistry, 71, 3–8.