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Supplementary Material

Experimental and Computational Approaches to Rationalise Multicomponent Supramolecular Assemblies: Dapsone Monosolvates

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1. Experimental Screen for DDS (Mono)Solvates

1.1 Solvent Evaporation Experiments

The evaporative crystallisation screen of **DDS** was designed from 35 pure solvents. Saturated solutions (at 25 °C) of DDS in the respective solvent were filtered and evaporation was conducted from watch glasses at room temperature. If the solubility was lower than 1mg per 1 mL then the solution was gently heated prior filtration.

The results of the evaporative crystallisation screen are summarised in Table S1. Solvate/hydrate forms were obtained from acetone, cyclohexanone, dichloromethane, dimethyl formamide, dimethyl sulfoxide,1,4-dioxane, methyl ethyl ketone, tetrahydrofuran and water. Evaporation experiments from other solvent solutions resulted in form III. All literature solvates and the hydrate were found in the evaporative crystallisation screen.

Table S1. Summary of Evaporative Crystallisation Experiments.

Solvent (volumes, mL/mg)	**Heating**	**Temp** (ºC)	**Morphology**	**Solid Form**[a] (PXRD)
Water (10/10)	yes	25	Elongated plates	III >> Hy
Methanol (2/25)		25	Elongated plates	III
Ethanol (8/28)		25	Plates	III
1-Propanol (>15/30)		25	Irregular plates	III
2-Propanol (>15/20)	yes	25	Irregular plates	III
1-Butanol (11/11)	yes	25	Grainy crystals	III
Iso-Butanol (10/9)	yes	25	Grainy crystals	III
1-Pentanol (10/9)	yes	25	Small, thin crystals	III
iso-Pentanol (10/9)	yes	25	Long platy crystals	III
t-Pentanol (12/12)	yes	25	Long platy crystals	III
Decanol (10/9)	yes	25		Practically insoluble
Methylene glycol (3.5/20)	yes	25		No crystallisation in 4 months
Propylene glycol (4/19)	yes	25	Platy crystals	III
Acetone (1/21)		25	Plates	III
Acetonitrile (<1/20)		25	Plates (desolvated)	III + S_{ACO}
Butyl acetate (>12/20)		25	Plates	III
Chloroform (>15/20)		25	Small platy crystals	III
Cyclohexane (>10/8)	yes	25		Practically insoluble
Cyclohexanone (5/20)		25	Dendrites	S_{CHOX}
Dichloromethane (>9/10)		25	Irregularly shapes plates (desolvated)	III + S_{DCM}
Diethyl ether (>20/18)		25	Platty crystals	III
Di-isopropyl ether (>13/13)	yes	25	Blocks	III
Dimethylformamide (>7/20)		25	Spherulithes (desolvated)	III > S_{DMF}
Dimethyl sulfoxide (<1/20)		25	Spherulithes (desolvated)	III > S_{DMSO}
1,4-Dioxane (>7/20)		25	Desolvated blocks and spherulithes	III (S_{DX})
Ethyl acetate (3.5/26)		25	Plates	III
Methyl ethyl ketone (<1/26)		25	Spherulithes (desolvated)	III (S_{MEK})
n-Heptane (10/8)	yes	25		Practically insoluble

Solvent (volumes, mL/mg)	Heating	Temp (ºC)	Morphology	Solid Form[a] (PXRD)
Methyl isobutyl ketone (3.5/20)		25	Spherulithes and grainy crystals	III
Methyl t-butyl ether (>12/10)	yes	25	Fine crystals, ? desolvated	III
Nitromethane (1.5/21)		25	Plates	III
Carbon tetrachloride (>10/10)	yes	25		Practically insoluble
Tetrahydrofuran (2.2/19)		25	Desolvated crystals and spherulithes	III (S_{THF})
Toluene (>10/10)	yes	25	Rectangular plates	III
Xylene	yes	25	Rectangular elongated plates	III

[a] **III** – form III, S_{ACO} – acetone solvate, S_{CHOX} – cyclohexanone solvate, S_{DCM} – dichloromethane solvate, S_{DMF} – dimethyl formamide solvate, S_{DMSO} – dimethyl sulfoxide solvate, S_{DX} – 1,4-dioxane solvate, S_{MEK} – methyl ethyl ketone solvate, S_{THF} – tetrahydrofuran solvate, **Hy** – 0.33-hydrate.

1.2 Cooling Crystallisation Experiments

The cooling crystallisation screen of **DDS** was designed from 29 solvents. Crystallisation experiments were conducted by natural cooling to 5 °C, RT, 50 °C and 75 °C.

The results of the cooling crystallisation screen are summarised in Table S2. In addition to the in the solvent evaporation experiments identified solvates, three additional DDS solvates emerged from the cooling crystallisation experiments: acetonitrile-, nitromethane- and carbon tetrachloride solvates. Furthermore, three transient solvates were identified (diethyl ether, di-isopropyl ether, methyl t-butyl ether). The lower the crystallisation temperature the more likely that the solvate will form. All other crystallisation experiments resulted in form III.

Table S2. Summary of Cooling Crystallisation Experiments.

Solvent	T_{cryst} (ºC)	Solid Form (HSM)	T_{cryst} (ºC)	Solid Form (HSM)	T_{cryst} (ºC)	Solid Form (HSM)	T_{cryst} (ºC)	Solid Form (HSM)
Water	5	Hy	RT	Hy	50	Hy	75	Hy
Methanol	5	III	RT	III	50	III		
Ethanol	5	III	RT	III	50	III		
1-Propanol	5	III	RT	III	50	III	75	III
2-Propanol	5	III	RT	III	50	III	75	III
1-Butanol	5	III	RT	III	50	III	75	III
iso-Butanol	5	III	RT	III	50	III	75	III
t- Butanol	5	III	RT	III	50	III	75	III
Acetone	5	S_{ACO}	RT	III + S_{ACO}				
Acetonitrile	5	S_{ACN}	RT	III + S_{ACN}	50	III	75	III
Butyl Acetate	5	III	RT	III	50	III	75	III
Chloroform	5	III	RT	III	50	III		
Cyclohexanone	5	S_{CHOX}	RT	III + S_{CHOX}	50	III	75	III
Dichloromethane	5	S_{DCM}	RT	S_{DCM}				
Diethyl ether	5	Solvate	RT	III				
Di-isopropyl ether	5	Solvate	RT	III				
DMF		III + S_{DMF}	RT	III + S_{DMF}	50	III	75	III
DMSO			RT	No crystallis.	50	No crystallis.	75	No crystallis.
1,4-Dioxane			RT	S_{DX}	50	S_{DX}	75	S_{DX}

Solvent	T_{cryst} (ºC)	Solid Form (HSM)	T_{cryst} (ºC)	Solid Form (HSM)	T_{cryst} (ºC)	Solid Form (HSM)	T_{cryst} (ºC)	Solid Form (HSM)
Ethyl Acetate	5	III	RT	III	50	III	75	III
Ethylene Chloride	5	III	RT	III	50	III	75	III
Methyl Ethyl Ketone	5	S_{MEK}	RT	III	50	III	75	III
Methyl i-Butyl Ketone			RT	III	50	III	75	III
Methyl t-Butyl Ether	5	Solvate	RT	III	50	III		
Nitromethane	5	S_{NM}	RT	S_{NM}	50	III	75	III
Tetrahydrofuran	5	S_{THF}	RT	S_{THF}	50	S_{THF}		
Carbon Tetrachloride			RT	S_{CTC}	50	S_{CTC} + III		
Toluene	5	III	RT	III	50	III	75	III
Xylene	5	III	RT	III	50	III	75	III

[a] **III** – form III, S_{ACO} – acetone solvate, S_{CHOX} – cyclohexanone solvate, S_{DCM} – dichloromethane solvate, S_{DMF} – dimethyl formamide solvate, S_{DX} – 1,4-dioxane solvate, S_{MEK} – methyl ethyl ketone solvate, S_{THF} – tetrahydrofuran solvate, S_{ACN} – acetonitrile solvate, S_{NM} – nitromethane solvate, S_{CTC} – carbon tetrachloride solvate, **Hy** – 0.33-hydrate.

1.3 Anti-solvent Addition Crystallisation Experiments

The antisolvent addition crystallisation screen of DDS was designed from 57 mixed solvent systems that were selected based on the requirements of solvent/anti-solvent miscibility, initial *vs*. final solubility in pure and mixed solvents. Standard (AA) and reverse anti-solvent addition (RAA) experiments were conducted at RT. The results of the anti-solvent addition crystallisation screen are summarised in Table S6. For all experiments 10 mg of DDS form III was used as starting material. With the exception of the acetonitrile (0.5) // di-isopropyl ether (9.5) anti-solvent addition all experiments resulted in form III.

Table S3. Summary of Anti-solvent Addition Crystallisation Experiments.

Solvent // Anti-solvent (volumes mL)	Method[a]	Temp (ºC)	Morphology	Solid Form[b] (PXRD)
Methanol (1.5) // Toluene (19.5)	AA	25	Plates	III
Ethanol (4) // Toluene (16)	AA	25		No crystallisation
Acetone (0.5) // Toluene (2.5)	AA	25	Plates	III
Acetonitrile (0.75) // Toluene (19.25)	AA	25	Plates, needles	III
Cyclohexanone (1.5) // Toluene (18.5)	AA	25		No crystallisation
Dimethyl formamide (0.5) // Toluene (14.5)	AA	25	Plates	III
Dimethyl sulfoxide (0.25) // Toluene (5)	AA	25		No crystallisation
Ethyl Acetate (1.5) // Toluene (18.5)	AA	25	Big blocks	III
Methyl ethyl ketone (0.5) // Toluene (4)	AA	25	Needles	III
Methyl isobutyl ketone (1.75) // Toluene (18)	AA	25		No crystallisation
Nitromethane (1) // Toluene (19)	AA	25	Plates	III
Tetrahydrofuran (1) // Toluene (10)	AA	25	Plates	III
Methanol (1.5) // 1-Butanol (13.5)	AA	25		No crystallisation
Ethanol (3.5) // 1-Butanol (6.5)	AA	25		No crystallisation
Acetone (0.5) // 1-Butanol (9.5)	AA	25	Plates	III
Acetonitrile (0.5) // 1-Butanol (9.5)	AA	25		No crystallisation
Cyclohexanone (1.5) // 1-Butanol (8.5)	AA	25		No crystallisation
Dimethyl formamide (0.5) // 1-Butanol (9.5)	AA	25		No crystallisation
Dimethyl sulfoxide (0.25) // 1-Butanol (4.75)	AA	25		No crystallisation
Ethyl acetate (1.5) // 1-Butanol (8.5)	AA	25		No crystallisation
Methyl ethyl ketone (0.5) // 1-Butanol (9.5)	AA	25		No crystallisation
Methyl isobutyl ketone (1.5) // 1-Butanol (8.5)	AA	25		No crystallisation
Nitromethane (1) // 1-Butanol (9)	AA	25		No crystallisation
Tetrahydrofuran (1) // 1-Butanol (9)	AA	25		No crystallisation
Methanol (1.5) // Di-isopropyl ether (8.5)	AA	25	Plates	III
Ethanol (3.5) // Di-isopropyl ether (6.5)	AA	25	Plates	III
Acetone (0.5) // Di-isopropyl ether (2.5)	AA	25	Irregular blocks	III
Acetonitrile (0.5) // Di-isopropyl ether (9.5)	AA	25	Needles	S_{ACN}
Cyclohexanone (1) // Di-isopropyl ether (3.5)	AA	25		No crystallisation
Dimethyl formamide (0.5) // Di-isopropyl ether (2)	AA	25		No crystallisation
Dimethyl sulfoxide (0.25) // Di-isopropyl ether (9)	AA	25		No crystallisation
Ethyl acetate (1.2) // Di-isopropyl ether (9)	AA	25	Plates	III
Methyl ethyl ketone (0.5) // Di-isopropyl ether (1)	AA	25		III
Methyl isobutyl ketone (1.5) // Di-isopropyl ether (8.5)	AA	25		III
Nitromethane (1) // Di-isopropyl ether (9)	AA	25		III
Tetrahydrofuran (1) // Di-isopropyl ether (4.5)	AA	25		III
Methanol (1) // Chloroform (5)	RAA	25	Irregular Plates	III
Methanol (1) // Butyl acetate (5)	RAA	25		No crystallisation

Solvent // Anti-solvent (volumes mL)	Method[a]	Temp (ºC)	Morphology	Solid Form[b] (PXRD)
Acetone (1) // Chloroform (5)	RAA	25	Big plates	III
Acetone (1) // Butyl acetate (5)	RAA	25		No crystallisation
Acetone (1) // Heptane (5)	RAA	25	Irregular plates	III
Acetone (1) // 1-Butanol (5)	RAA	25		No crystallisation
Acetonitrile (0.5) // Chloroform (5)	RAA	25		No crystallisation
Acetonitrile (0.5) // Butyl acetate (5)	RAA	25		No crystallisation
Acetonitrile (0.5) // 1-Butanol (5)	RAA	25	Plates	III
Ethyl Acetate (1.2) // Chloroform (5)	RAA	25	Plates	III
Ethyl Acetate (1.2) // Butyl acetate (5)	RAA	25		No crystallisation
Ethyl Acetate (1.2) // Heptane (5)	RAA	25	Irregular plates	III
Ethyl Acetate (1.2) // 1-Butanol (5)	RAA	25		No crystallisation
Nitromethane (1) // Chloroform (5)	RAA	25	Small plates	III
Nitromethane (1) // Butyl acetate (5)	RAA	25	Plates	III
Nitromethane (1) // Heptane (5)	RAA	25	Needles	III
Nitromethane (1) // 1-Butanol (5)	RAA	25		No crystallisation
Dimethyl sulfoxide (0.1) // Toluene (5)	RAA	25		No crystallisation
Dimethyl sulfoxide (0.1) // Heptane (5)	RAA	25		No crystallisation
Dimethyl sulfoxide (0.1) // Di-isiopropyl ether (5)	RAA	25		No crystallisation
Dimethyl sulfoxide (0.1) // Butyl acetate (5)	RAA	25		No crystallisation

[a] AA – anti-solvent addition, RAA – reverse anti-solvent addition; [b] **III** – form III, S_{ACN} – acetonitrile solvate.

1.4 Solvent Evaporation Experiments – Mixed Solvents

The (reverse) anti-solvent addition experiments which did not crystallise within 6 weeks were transferred onto watch glasses and evaporation was conducted at room temperature. Form III and the nitromethane solvate emerged from the experiments.

Table S4. Summary of Evaporative Crystallisation Experiments 2.

Solvent mixture (volumes mL)	Temp (ºC)	Solid Form[a] (PXRD / HSM)
Ethanol (4) // Toluene (16)	25	III
Cyclohexanone (1.5) // Toluene (18.5)	25	III
Dimethyl sulfoxide (0.25) // Toluene (5)	25	III
Methyl isobutyl ketone (1.75) // Toluene (18)	25	III
Methanol (1.5) // 1-Butanol (13.5)	25	III
Ethanol (3.5) // 1-Butanol (6.5)	25	III
Acetonitrile (0.5) // 1-Butanol (9.5)	25	III
Cyclohexanone (1.5) // 1-Butanol (8.5)	25	III
Dimethyl formamide (0.5) // 1-Butanol (9.5)	25	III
Dimethyl sulfoxide (0.25) // 1-Butanol (4.75)	25	III

Solvent mixture (volumes mL)	Temp (ºC)	Solid Form[a] (PXRD / HSM)
Ethyl acetate (1.5) // 1-Butanol (8.5)	25	III
Methyl ethyl ketone (0.5) // 1-Butanol (9.5)	25	III
Methyl isobutyl ketone (1.5) // 1-Butanol (8.5)	25	III
Nitromethane (1) // 1-Butanol (9)	25	S_{NM}
Tetrahydrofuran (1) // 1-Butanol (9)	25	III
Cyclohexanone (1) // Di-isopropyl ether (3.5)	25	III
Dimethyl formamide (0.5) // Di-isopropyl ether (2)	25	III
Dimethyl sulfoxide (0.25) // Di-isopropyl ether (9)	25	III
Methanol (1) // Butyl acetate (5)	25	III
Acetone (1) // Butyl acetate (5)	25	III
Acetone (1) // 1-Butanol (5)	25	III
Acetonitrile (0.5) // Chloroform (5)	25	III
Acetonitrile (0.5) // Butyl acetate (5)	25	III
Ethyl Acetate (1.2) // Butyl acetate (5)	25	III
Ethyl Acetate (1.2) // 1-Butanol (5)	25	III
Nitromethane (1) // 1-Butanol (5)	25	III
Dimethyl sulfoxide (0.1) // Toluene (5)	25	III
Dimethyl sulfoxide (0.1) // Heptane (5)	25	III
Dimethyl sulfoxide (0.1) // Di-isopropyl ether (5)	25	III
Dimethyl sulfoxide (0.1) // Butyl acetate (5)	25	III

[a] III – form III, S_{NM} – nitromethane solvate.

1.5 Slurry Experiments

Suspension of DDS in 36 organic solvents were stirred in between 10 and 20 °C. Samples were withdrawn periodically and the residue analysed with PXRD. The solvent bridging experiments produced elven solvate forms of DDS (Table S5).

Table S5. Summary of Solvent Slurry Experiments.

Solvent	Solid Form[a] (PXRD)	Solvent	Solid Form[a] (PXRD)
Water	Hy	Cyclohexanone	S_{CHOX}
Methanol	III + V	Dichloromethane	S_{DCM}
Ethanol	III < V	Diethyl ether	V + Hy / S (III) + V[b]
1-Propanol	III	Di-isopropyl ether	III / S (III)[b]
2- Propanol	III	Dimethylformamide	S_{DMF}
1-Butanol	III	Dimethyl sulfoxide	sticky paste
iso- Butanol	III	1,4-Dioxane	S_{DX}
1-Pentanol	III	Ethyl acetate	III
iso- Pentanol	III	Methyl ethyl ketone	S_{MEK}
t- Pentanol	III	n-Heptane	III + Hy
Decanol	V	Methyl isobutyl ketone	V
Methylene Glycol	III	Methyl t-butyl ether	Hy / S (III)[b]
Propylene Glycol	III	Nitromethane	S_{NM}
Acetone	S_{ACO}	Carbon Tetrachloride	S_{CTC}
Acetonitrile	S_{ACN}	Tetrahydrofuran	S_{THF}
Butyl Acetate	III < V	Toluene	III
Chloroform	III + V	Xylene	V + Hy
Cyclohexane	III + V	1,2-Dichloroethane	S_{DCE}

[a] **III** – form III, V – form V, Hy – 0.33-hydrate, S_{ACO} – acetone solvate, S_{ACN} – acetonitrile solvate, S_{CHOX} – cyclohexanone solvate, S_{DCM} – dichloromethane solvate, S_{DMF} – dimethyl formamide solvate, S_{DX} – 1,4-dioxane solvate, S_{MEK} – methyl ethyl ketone solvate, S_{NM} – nitromethane solvate, S_{CTC} – carbon tetrachloride solvate, S_{THF} – tetrahydrofuran solvate, S_{DCE} – 1,2-dichloroethane solvate. [b] experiments were repeated using “water”-free solvents.

2. Systematic Storage-Stability Studies

An overview of the desolvation and storage stability studies performed is given in Table S6. The resulting DDS solid form was analysed at room temperature using PXRD. The only neat form obtained in the experiments was form III.

At higher relative humidities a transformation to the 0.33-hyrate was observed.

S$_{CHOX}$ was identified to be the solvate showing the "slowest" transformation rate.

Table S6. Overview of systematic desolvation and storage stability experiments of DDS solvates.

Temperature/ Heating rate (HR)/ Relative humidity	Time	**S$_{CTC}$**	**S$_{ACO}$**	**S$_{CHOX}$**	**S$_{DMF}$**	**S$_{THF}$**	**S$_{DCE}$**	**S$_{MEK}$**	**S$_{DX}$**
Temperature dependent, ambient RH (30% RH)									
25 °C	24 hours	III	III	S < III	S < III	S << III	III	III	III
25 °C	2 weeks	III	III	III	III	III	III	III	III
50 °C	24 hours	III	III	S << III	III	III	III	III	III
50 °C	1 week	III	III	III	III	III	III	III	III
75 °C	24 hours	III	III	III	III	III	III	III	III
75 °C	1 week	III	III	III	III	III	III	III	III
Temperature dependent, 0% RH									
25 °C	24 hours	S < III	III	S < III	S << III	S << III	III	III	S << III
25 °C	2 weeks	III	III	III	III	III	III	III	III
50 °C	24 hours	III	III	S < III	III	III	III	III	III
50 °C	1 week	III	III	III	III	III	III	III	III
75 °C	24 hours	III	III	III	III	III	III	III	III
75 °C	1 week	III	III	III	III	III	III	III	III
Vacuum									
25 °C	48 hours	III	III	III	III	III	III	III	III
TGA, N_2 purge									
HR 10 °C min^{-1}		III	III	Liq.	n.a.	III	III	III	III
HR 5 °C min^{-1}		III	III	Liq.	III	III	III	III	III
HR 2 °C min^{-1}		III	III	Liq.	III	III	III	III	III
HR 1 °C min^{-1}		n.a.	n.a.	n.a.	III	n.a.	n.a.	n.a.	n.a.
DSC, hermetically sealed pan									
HR 10 °C min^{-1}		III	III	Liq.	III	III	III	III	S + III (stopped at 140 °C)
Moisture dependent, 25 °C									
24% RH	6 days	III	III	S > III	S << III	III	III	III	III
43% RH	6 days	III	III	S and III	S < III	III	III	III	III
75% RH	6 days	III	III > Hy	S + III + Hy	III	III > Hy	III > Hy	III + Hy	III + Hy
100% RH	6 days	III > Hy	Hy	S + III + Hy	Hy	Hy	III < Hy	III + Hy	III + Hy

III – Form III; S – Solvate; Hy – 0.33-Hydrate; Liq. – liquid (DDS dissolved in CHOX); n.a. – not attempted.

3. Monosolvate Crystal Structure Models

Structural insights into the packing of the six new monosolvates of DDS (**S**$_{\text{CTC}}$, **S**$_{\text{ACO}}$, **S**$_{\text{CHOX}}$, **S**$_{\text{DMF}}$, **S**$_{\text{MEK}}$ and **S**$_{\text{DCE}}$) was achieved as follows:

1. Solvate forms were prepared *via* slurry experiments of DDS in the respective solvent and the temperature was cycled between 10 and 20 °C. Within hours the transformation to the solvates occurred.
2. The recorded PXRD patterns (between two mylar foils to slow down/prevent desolvation, measured at RT) were indexed and Pawley fitting was used to derive the room temperature lattice parameters.
3. Solvate stoichiometries were estimated based on (1) the cell volume of the solvates and (2) using thermogravimetric analysis (TGA).
4. Crystal structure prediction (CSP) searches were performed to generate hypothetical low energy monosolvate structures, with the lattice energy being calculated at the PBE-TS and PBE-D2 level of theory.
5. The experimental PXRD patterns were compared to the PXRD patterns simulated from the computationally generated structures in step 4.
6. Closet matching structures were optimised using the experimental RT lattice parameters (*i.e.*, fixed cell) and the atomic positions were optimised.
7. Rigid-body Rietveld refinements, using the in step 6 minimised structures as starting models, were performed.
8. Structures obtained from the Rietveld refinements were optimised again to confirm the correctness of the model.

3.1. Step 2: Pawley fitting

Table S7 list the refined RT lattice parameters of the DDS solvates and form III and Figure S1 to Figure S9 show the Pawley fits.

Table S7. Unit cell parameters and space group symmetry derived from indexation of DDS solvate RT PXRD patterns.

Solid Form	SG	a / Å	b / Å	c / Å	alpha	beta	gamma	Volume / Å^3	R_{exp}	R_{wp}	R_p
Anhydrate											
Form **III**	$P2_12_12_1$	5.7501(<1)	8.0472(<1)	25.4957(3)	90	90	90	1179.73(2)	*3.65*	*3.95*	*3.04*
Hemi-Solvates											
S-Acetonitrile (**S$_{ACN}$**)	$P2_1/c$	8.5352(2)	16.3078(4)	22.2536(7)	90	120.500(1)	90	2668.87(14)	1.49	6.04	3.69
S-Nitromethane (**S$_{NM}$**)	$P2_1/c$	8.4638(3)	16.2489(7)	22.8563(9)	90	120.578(<1)	90	2705.71(19)	1.50	3.21	4.26
S-Dichloromethane (**S$_{DCM}$**)	$P2_1/c$	8.3560(2)	16.6089(4)	20.5183(7)	90	104.250(1)	90	2759.99(15)	1.65	3.10	1.91
Mono-Solvates											
S-Carbon tetrachloride (**S$_{CCl4}$**)	$P2_1$	8.7408(1)	17.4109(2)	5.7875(<1)	90	104.812(<1)	90	851.51(2)	2.98	3.36	2.52
S-Acetone (**S$_{ACO}$**)	$P2_1/c$	5.9775(1)	12.4298(3)	22.4392(6)	90	104.068(1)	90	1617.07(8)	1.65	7.35	5.79
S-Cyclohexanone (**S$_{CHXO}$**)	$P2_1/c$	6.0749(<1)	13.7461(2)	22.5823(3)	90	106.307(<1)	90	1809.90(4)	1.42	2.72	1.57
S-Dimethyl formamide (**S$_{DMF}$**)	$P2_1/c$	6.1019(1)	12.6882(3)	22.4029(5)	90	108.004(<1)	90	1649.54(7)	8.74	8.26	5.93
S-Tetrahydrofuran (**S$_{THF}$**)	$P2_1/c$	5.9003(1)	12.8549(1)	22.5182(2)	90	104.132(1)	90	1656.26(3)	1.71	4.20	3.63
S-Methyl ethyl ketone (**S$_{MEK}$**)	*Pbca*	8.6083(1)	16.3216(3)	25.0261(5)	90	90	90	3516.20(11)	1.55	4.53	3.68
S-Dichloroethane (**S$_{DCE}$**)	*Pbca*	8.6757(1)	16.7576(2)	23.1301(3)	90	90	90	3362.74(8)	1.32	2.23	1.68
S-Dioxane (**S$_{DX}$**)	*Pbca*	11.4025(6)	11.3964(5)	26.3041(15)	90	90	90	3418.15(32)	8.61	9.81	7.80

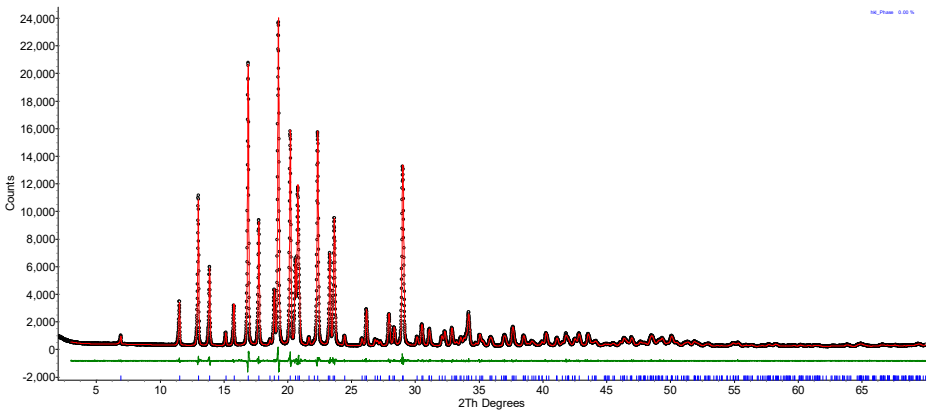


Figure S1. Pawley fit between the PXRD data of form III with a model consisting of the cell parameters derived from indexing the PXRD pattern. Black dots indicate the raw data, while the red line indicates the calculated model. Tick marks (blue) are the 2θ positions for the *hkl* reflections. The difference pattern is shown in green.

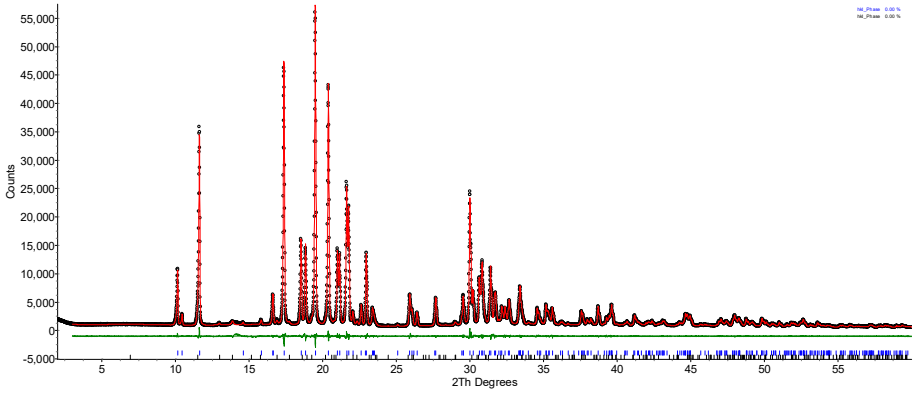


Figure S2. Pawley fit between the PXRD data of Carbon Tetrachloride Monosolvate with a model consisting of the cell parameters derived from indexing the PXRD pattern (note that form III impurities are present). Black dots indicate the raw data, while the red line indicates the calculated model. Tick marks (blue – solvate and black – form III) are the 2θ positions for the *hkl* reflections. The difference pattern is shown in green.

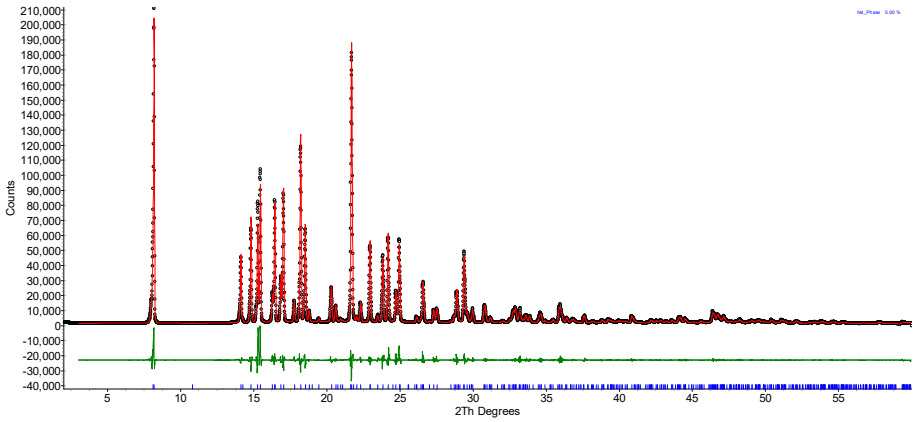


Figure S3. Pawley fit between the PXRD data of Acetone Monosolvate with a model consisting of the cell parameters derived from indexing the PXRD pattern. Black dots indicate the raw data, while the red line indicates the calculated model. Tick marks are the 2θ positions for the *hkl* reflections. The difference pattern is shown in green.

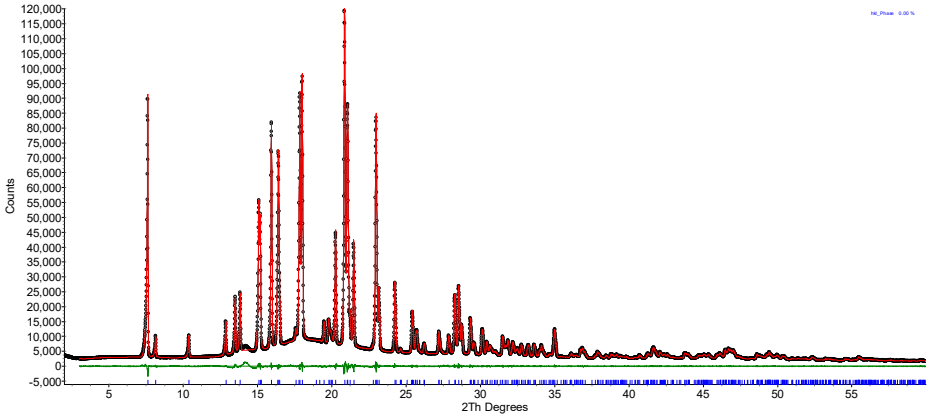


Figure S4. Pawley fit between the PXRD data of Cycolhexanone Monosolvate with a model consisting of the cell parameters derived from indexing the PXRD pattern. Black dots indicate the raw data, while the red line indicates the calculated model. Tick marks are the 2θ positions for the *hkl* reflections. The difference pattern is shown in green.

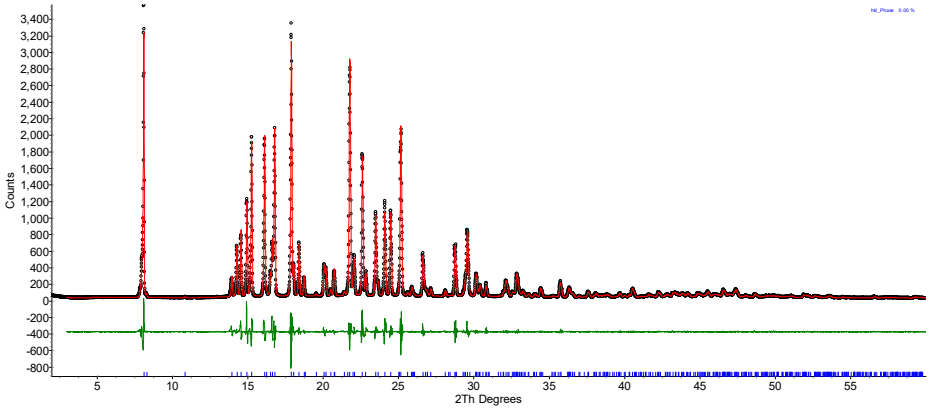


Figure S5. Pawley fit between the PXRD data of DMF Monosolvate with a model consisting of the cell parameters derived from indexing the PXRD pattern. Black dots indicate the raw data, while the red line indicates the calculated model. Tick marks are the 2θ positions for the *hkl* reflections. The difference pattern is shown in green.

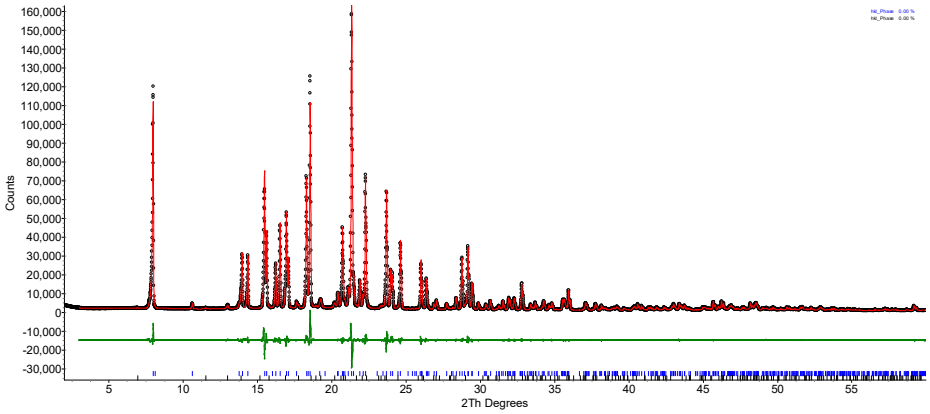


Figure S6. Pawley fit between the PXRD data of Tetrahydrofuran Monosolvate with a model consisting of the cell parameters derived from indexing the PXRD pattern (note that form III impurities are present). Black dots indicate the raw data, while the red line indicates the calculated model. Tick marks (blue – solvate and black – Form III) are the 2θ positions for the *hkl* reflections. The difference pattern is shown in green.

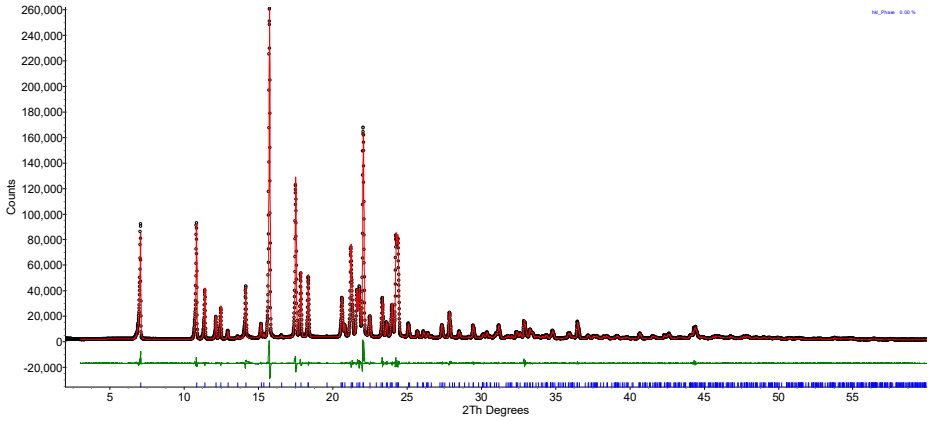


Figure S7. Pawley fit between the PXRD data of Methyl Ethyl Ketone Monosolvate with a model consisting of the cell parameters derived from indexing the PXRD pattern. Black dots indicate the raw data, while the red line indicates the calculated model. Tick marks are the 2θ positions for the *hkl* reflections. The difference pattern is shown in green.

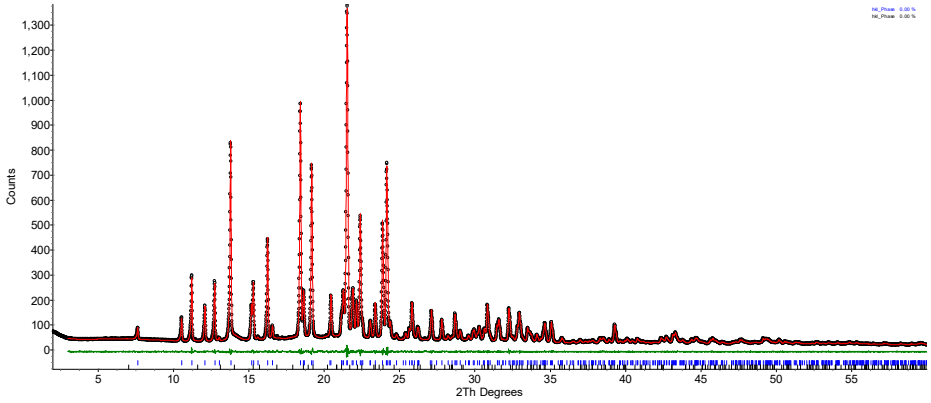


Figure S8. Pawley fit between the PXRD data of DCE Monosolvate with a model consisting of the cell parameters derived from indexing the PXRD pattern. Black dots indicate the raw data, while the red line indicates the calculated model. Tick marks are the 2θ positions for the *hkl* reflections. The difference pattern is shown in green.

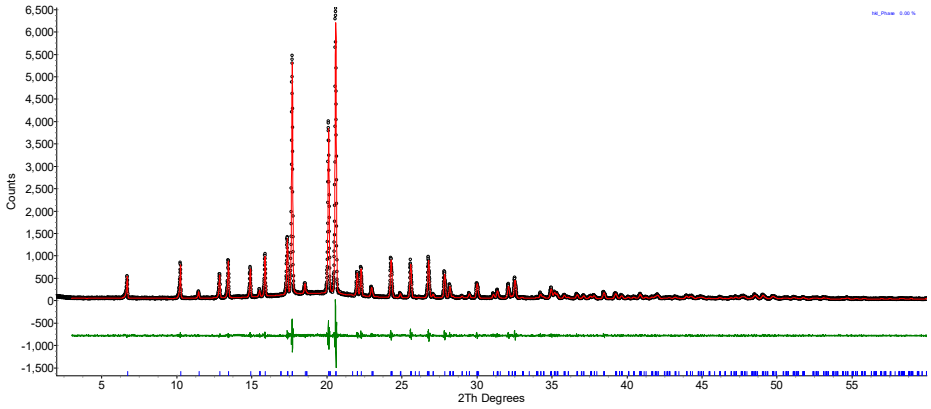


Figure S9. Pawley fit between the PXRD data of 1,4-Dioxane Monosolvate with a model consisting of the cell parameters derived from indexing the PXRD pattern. Black dots indicate the raw data, while the red line indicates the calculated model. Tick marks the 2θ positions for the *hkl* reflections. The difference pattern is shown in green.

3.2. Steps 5 and 6: Comparison of Experimental and Computed Structures

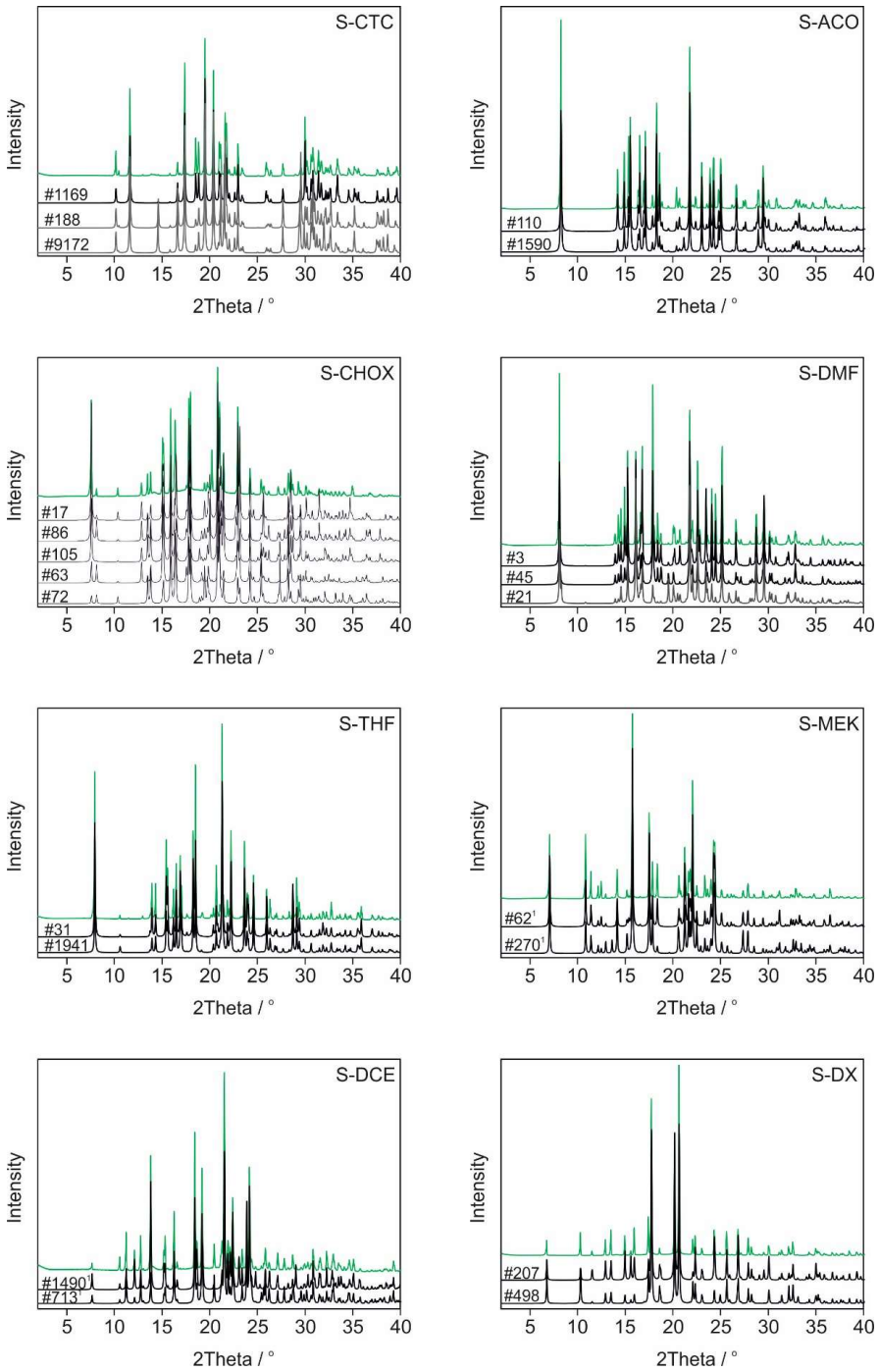


Figure S10. Comparison of experimental and simulated (form computationally generated structures, with lattice parameters fixed to RT values, labelled with #..) DDS solvate PXRD patterns.

3.3. Step 7: Rietveld Refinement

The minimised structures (step 6) were used as an input for Rietveld refinements, 2θ range 3.0 to 60.0°, using TOPAS academic V5.[1] The geometry of each molecule was defined by a rigid body. Rotation and translation parameters were simultaneously refined with the SO_2–phenyl dihedrals of DDS. The background was modelled by a set of consecutive points with refineable intensities.

Table S8. Summary of Rietveld refinements

	S_{CTC}	S_{ACO}	S_{CHOX}	S_{DMF}	S_{MEK}	S_{DCE}
Measurement Conditions						
	Cu $K_{\alpha1,2}$	Cu $K_{\alpha1,2}$	Cu $K_{\alpha1,2}$	Cu $K_{\alpha1,2}$	Cu $K_{\alpha1,2}$	Cu $K_{\alpha1,2}$
2θ range	3.00-59.99	3.00-59.88	3.00-59.8	3.00-59.88	3.00-59.88	3.00-59.99
excluded 2θ range	13.45-14.48	–	14.00-14.60	–	–	13.95-14.62
data points	8287	8287	8287	8287	8287	8287
Measurements	45 x 40 s	20 x 40 s	32 x 40 s	45 x 40 s	17 x 40 s	45 x 40 s
Crystal Data						
space Group	$P2_1$	$P2_1/n$	$P2_1/n$	$P2_1/n$	*Pbca*	*Pbca*
a / Å	5.7874(<1)	5.9769(<1)	6.0746(1)	6.1023(1)	8.6085(1)	8.6756
b / Å	17.4106(2)	12.7288(3)	13.7444(3)	12.6884(4)	16.3204(2)	16.7580
c / Å	8.7403(<1)	21.7679(3)	21.6710(4)	21.3230(5)	25.0267(5)	23.1266
β / °	104.810(<1)	91.344(1)	90.707(<1)	92.208(8)	90	90
V / $Å^3$	851.46(1)	1616.60(5)	1809.20(7)	1649.80(8)	3516.10(11)	3362.26(12)
Refinement						
phases[a]	S and Form III	S	S	S	S	S and Form III
solvent molecule	2 positions	2 positions	2 positions	2 positions	2 positions	2 positions
solvent disorder ratio	0.60:0.40	0.70:0.30	0.78:0.22	0.60:0.40	0.77:0.23	0.57:0.43
Parameters	80	63	93	69	69	79
Profile	28	25	58	32	3	32
Cell	4 + 3	4	4	4	4	3
Scale	1 + 1	1	1	1	1	1
preferred orientation	14 + 6	11	10	10	10	10
B_{iso}	C,N,O,S: 3.62(7) H: 1.2*3.62(7) Cl: 7.84(7)	4.52(9) 1.2*4.52(9)	6.00(13) 1.2*6.00(13)	6.26(14) 1.2*6.26(14)	6.00(10) 1.2*6.00(10)	6.00(12) 1.2*6.00(12) 10.80(18)
Positions	20	20	18	20	20	20
occupancy (disorder)	1	1	1	1	1	1
R_{wp} / %	5.24	10.18	6.90	10.37	8.31	6.42
R_{exp} / %	2.19	2.01	1.49	2.01	2.09	1.53
R_p / %	3.79	7.54	4.65	7.86	6.07	4.60
refine_ls_shift/su_max	<0.001	0.020	0.009	0.0008	0.018	0.009

[a]S – solvate

PXRD patterns were recorded using an X'Pert PRO diffractometer (PANalytical, Almelo, the Netherlands) equipped with a θ/θ coupled goniometer in transmission geometry, a Cu-$K_{\alpha1,2}$ radiation source with a focusing 0.5° divergence slit and 0.02° Soller slit collimator on the incident beam side, a 2 mm antiscattering slit and 0.04° Soller slit collimator on the diffracted beam side mirror, and a solid-state PIXcel detector. The patterns were recorded at a tube voltage of 40 kV and tube current of 40 mA, applying a step size of $2\theta = 0.013°$ with 45 times 40 s per step in the 2θ range between 2 and 60°.

The samples were measured between to foils to prevent/slow-down the desolvation of the solvates to form III. Only the PXRD patterns where no (or hardly any) form III reflections were detectable were used for the Rietveld refinements.

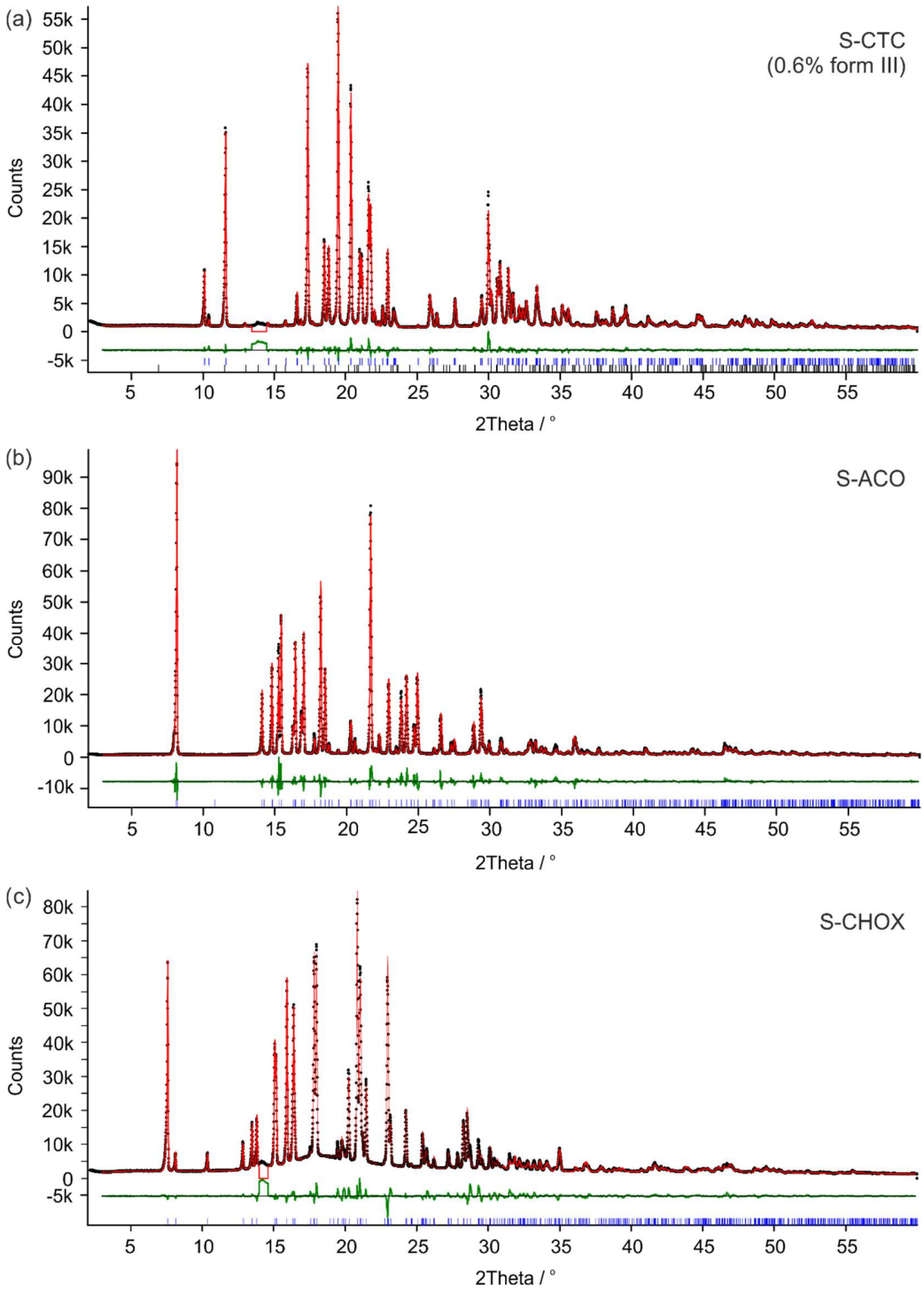


Figure S11. Observed (black points), calculated (red line) and difference (green line) profiles for the Rietveld refinement of (a) **S**$_{\mathbf{CTC}}$, (b) **S**$_{\mathbf{ACO}}$, and (c) **S**$_{\mathbf{CHOX}}$. Blue and black tick marks denote the solvate and form III peak positions, respectively.

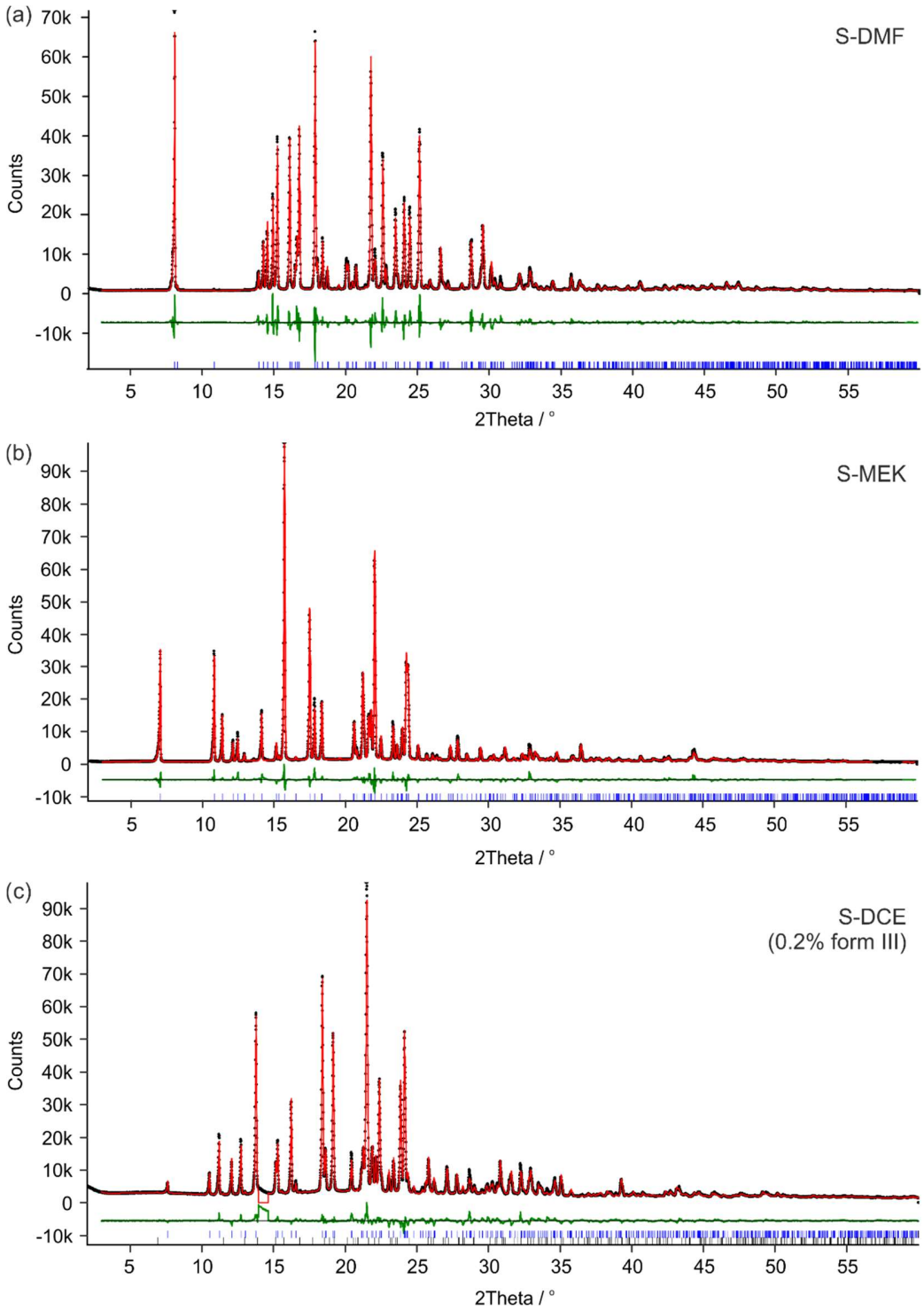


Figure S12. Observed (black points), calculated (red line) and difference (green line) profiles for the Rietveld refinement of (a) **S**$_{DMF}$, (b) **S**$_{MEK}$, and (c) **S**$_{DCE}$. Blue and black tick marks denote the solvate and form III peak positions, respectively.

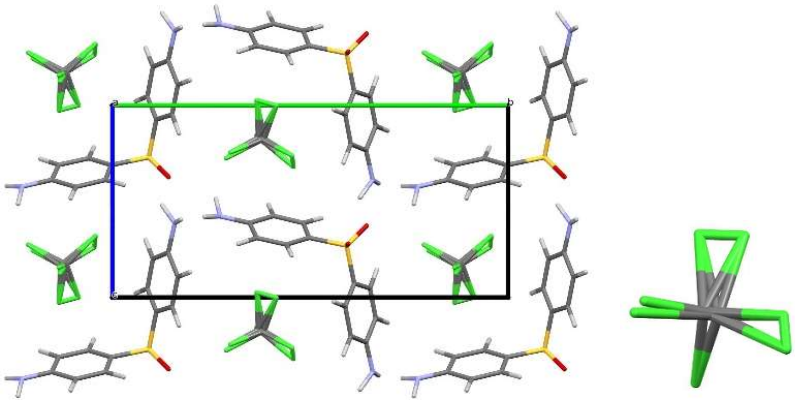


Figure S13. Carbon tetrachloride solvate: packing diagram (along *a*) and enlarged solvent molecule disorder over two positions.

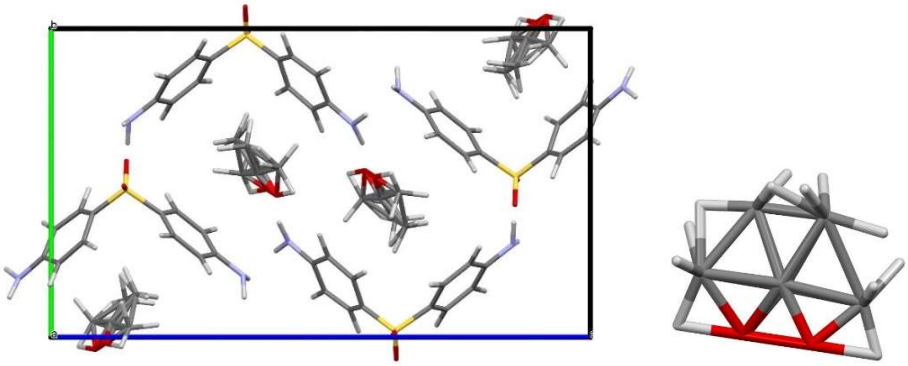


Figure S14. Acetone solvate: packing diagram (along *a*) and enlarged solvent molecule disorder over two positions.

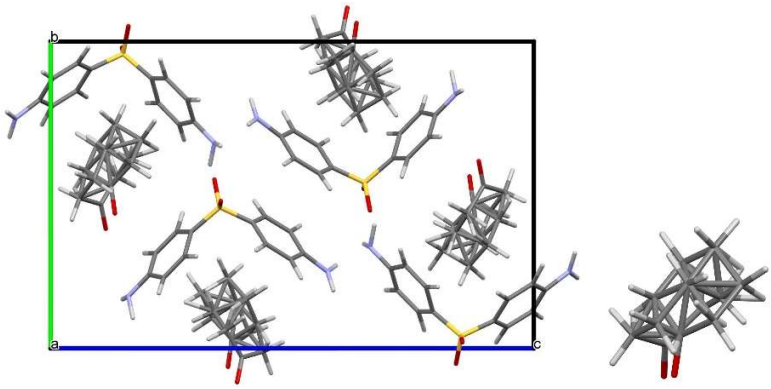


Figure S15. Cyclohexanone solvate: packing diagram (along *a*) and enlarged solvent molecule disorder over two positions.

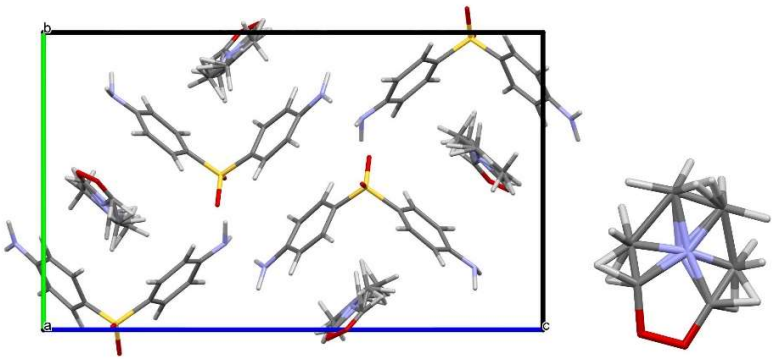


Figure S16. Dimethyl formamide solvate: packing diagram (along *a*) and enlarged solvent molecule disorder over two positions.

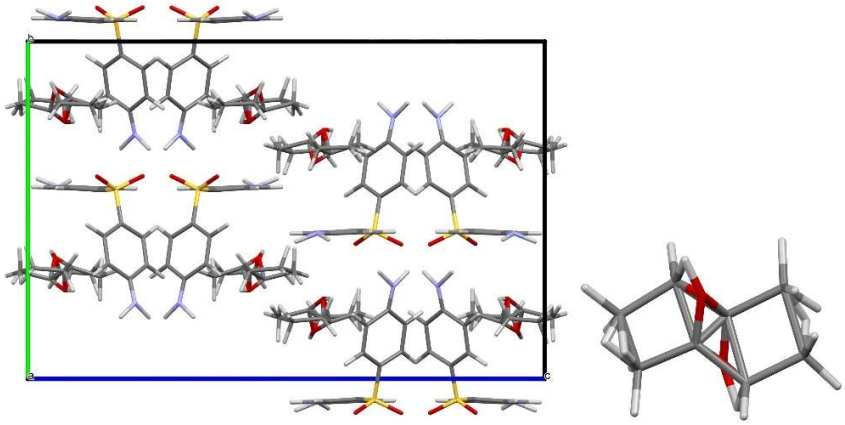


Figure S17. Methyl ethyl ketone solvate: packing diagram (along *a*) and enlarged solvent molecule disorder over two positions.

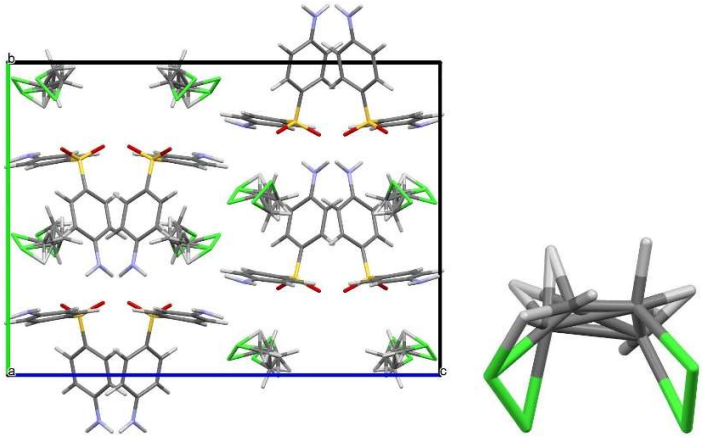


Figure S18. 1,2-Dichloroethane solvate: packing diagram (along *a*) and enlarged solvent molecule disorder over two positions.

3.4. Experimental Res Files

3.4.1. Carbon Tetrachloride Solvate

```
TITL CTC-Solvate
CELL 0.71073 5.78743 17.4106 8.74053 90 104.811 90
ZERR 2 0.000000 0.00000 0.000000 0 0.0000 0
LATT -1
SYMM -x,1/2+y,-z
SFAC C H N O S Cl
UNIT 28 24 4 4 2 16
FVAR 1.00
C1     1  0.546285  1.602456  1.201245  1.000000 0.045834
C2     1  0.767675  1.640939  1.233855  1.000000 0.045834
C3     1  0.420762  1.588372  1.046532  1.000000 0.045834
C4     1  0.857926  1.665383  1.107094  1.000000 0.045834
C5     1  0.733485  1.650702  0.952403  1.000000 0.045834
C6     1  0.505990  1.611045  0.926568  1.000000 0.045834
C7     1  0.414134  1.496974  0.689287  1.000000 0.045834
C8     1  0.280608  1.439648  0.724341  1.000000 0.045834
C9     1  0.324288  1.364455  0.690095  1.000000 0.045834
C10    1  0.503418  1.346744  0.612208  1.000000 0.045834
C11    1  0.642081  1.407272  0.575504  1.000000 0.045834
C12    1  0.600494  1.482330  0.612161  1.000000 0.045834
H1     2  0.861473  1.625912  1.479167  1.000000 0.055001
H2     2  1.067386  1.672515  1.405983  1.000000 0.055001
H3     2  0.411639  1.233454  0.580001  1.000000 0.055001
H4     2  0.623930  1.261714  0.487558  1.000000 0.055001
H5     2  0.473423  1.583947  1.298551  1.000000 0.055001
H6     2  0.248761  1.559235  1.022287  1.000000 0.055001
H7     2  1.028840  1.695477  1.131428  1.000000 0.055001
H8     2  0.806903  1.668118  0.855062  1.000000 0.055001
H9     2  0.138134  1.452730  0.780735  1.000000 0.055001
H10    2  0.217481  1.318393  0.721268  1.000000 0.055001
H11    2  0.783284  1.394593  0.517574  1.000000 0.055001
H12    2  0.712179  1.528272  0.586692  1.000000 0.055001
N1     3  0.890990  1.657965  1.387712  1.000000 0.045834
N2     3  0.544768  1.272119  0.577423  1.000000 0.045834
O1     4  0.094659  1.595956  0.720392  1.000000 0.045834
O2     4  0.444679  1.642198  0.626492  1.000000 0.045834
S1     5  0.350143  1.591941  0.729963  1.000000 0.045834
C13    1  0.047304  1.384612  0.173224  0.401151 0.045834
Cl1    6 -0.168876  1.414617  0.001006  0.401151 0.099330
Cl2    6 -0.053724  1.298669  0.244432  0.401151 0.099330
Cl3    6  0.320952  1.367350  0.125250  0.401151 0.099330
Cl4    6  0.086167  1.457341  0.319571  0.401151 0.099330
C13b   1  0.036759  1.367916  0.167344  0.598849 0.045834
Cl1b   6 -0.154400  1.364764 -0.026578  0.598849 0.099330
Cl2b   6 -0.025208  1.287420  0.275197  0.598849 0.099330
Cl3b   6  0.336881  1.364332  0.156518  0.598849 0.099330
Cl4b   6 -0.013920  1.454130  0.261709  0.598849 0.099330
END
```

3.4.2. Acetone Solvate

```
TITL DDS_Acetone Solvate
CELL 0.71073 5.97688 12.4288 21.7679 90 91.3445 90
ZERR 4 0.00010 0.0003 0.0003 0 0.0010 0
LATT 1
SYMM 1/2-x,1/2+y,1/2-z
SFAC C H N O S
UNIT 72 96 8 16 4
FVAR 1.00
C1     1 -0.070000  0.400000  0.205000  1.000000 0.057246
C2     1  0.150000  0.410000  0.232000  1.000000 0.057246
C3     1  0.200000  0.340000  0.282000  1.000000 0.057246
C4     1  0.050000  0.270000  0.305000  1.000000 0.057246
C5     1 -0.170000  0.260000  0.277000  1.000000 0.057246
C6     1 -0.220000  0.330000  0.227000  1.000000 0.057246
C7     1 -0.050000  0.400000  0.077000  1.000000 0.057246
C8     1 -0.170000  0.310000  0.060000  1.000000 0.057246
C9     1 -0.090000  0.240000  0.014000  1.000000 0.057246
C10    1  0.110000  0.260000 -0.014000  1.000000 0.057246
C11    1  0.240000  0.350000  0.007000  1.000000 0.057246
C12    1  0.170000  0.410000  0.054000  1.000000 0.057246
HN1A   2  0.010000  0.130000  0.358000  1.000000 0.068772
HN1B   2  0.260000  0.190000  0.365000  1.000000 0.068772
HN2A   2  0.330000  0.220000 -0.083000  1.000000 0.068772
HN2B   2  0.090000  0.130000 -0.077000  1.000000 0.068772
H2     2  0.280000  0.460000  0.215000  1.000000 0.068772
H3     2  0.370000  0.350000  0.304000  1.000000 0.068772
H5     2 -0.290000  0.210000  0.294000  1.000000 0.068772
H6     2 -0.390000  0.330000  0.205000  1.000000 0.068772
H8     2 -0.330000  0.290000  0.081000  1.000000 0.068772
H9     2 -0.190000  0.170000 -0.002000  1.000000 0.068772
H11    2  0.400000  0.370000 -0.014000  1.000000 0.068772
H12    2  0.270000  0.480000  0.070000  1.000000 0.068772
N1     3  0.090000  0.200000  0.356000  1.000000 0.057246
N2     3  0.190000  0.190000 -0.060000  1.000000 0.057246
O1     4  0.000000  0.570000  0.140000  1.000000 0.057246
O2     4 -0.370000  0.490000  0.135000  1.000000 0.057246
S1     5 -0.130000  0.480000  0.138000  1.000000 0.057246
C1sa   1  0.180000  0.140000  0.158000  0.698000 0.057246
C2sa   1  0.210000  0.050000  0.111000  0.698000 0.057246
C3sa   1  0.430000  0.050000  0.078000  0.698000 0.057246
H1sa   2  0.010000  0.130000  0.177000  0.698000 0.068772
H2sa   2  0.300000  0.130000  0.195000  0.698000 0.068772
H3sa   2  0.200000  0.220000  0.137000  0.698000 0.068772
H4sa   2  0.440000 -0.030000  0.052000  0.698000 0.068772
H5sa   2  0.430000  0.120000  0.046000  0.698000 0.068772
H6sa   2  0.570000  0.060000  0.110000  0.698000 0.068772
O1sa   4  0.060000 -0.020000  0.100000  0.698000 0.057246
C1sb   1  0.390000  0.120000  0.138000  0.302000 0.057246
C2sb   1  0.220000  0.030000  0.118000  0.302000 0.057246
C3sb   1 -0.010000  0.030000  0.145000  0.302000 0.057246
H1sb   2  0.540000  0.110000  0.114000  0.302000 0.068772
H2sb   2  0.310000  0.200000  0.130000  0.302000 0.068772
H3sb   2  0.420000  0.110000  0.188000  0.302000 0.068772
H4sb   2 -0.110000 -0.030000  0.130000  0.302000 0.068772
H5sb   2  0.000000  0.040000  0.196000  0.302000 0.068772
H6sb   2 -0.090000  0.110000  0.131000  0.302000 0.068772
O1sb   4  0.270000 -0.040000  0.082000  0.302000 0.057246
END
```

3.4.3. Cyclohexanone Solvate

```
TITL Cyclohexanone
CELL 0.71073 6.07456 13.7444 21.671 90 90.7067 90
ZERR 4 0.00012 0.0003 0.0004 0 0.0010 0
LATT 1
SYMM 1/2-x,1/2+y,1/2-z
SFAC C H N O S
UNIT 96 128 8 16 4
FVAR 1.00
C1     1  0.280000  0.300000  0.277000  1.000000 0.075991
C2     1  0.330000  0.230000  0.234000  1.000000 0.075991
C3     1  0.540000  0.240000  0.204000  1.000000 0.075991
C4     1  0.680000  0.310000  0.217000  1.000000 0.075991
C5     1  0.630000  0.380000  0.261000  1.000000 0.075991
C6     1  0.430000  0.380000  0.291000  1.000000 0.075991
C7     1  0.460000  0.410000  0.418000  1.000000 0.075991
C8     1  0.670000  0.430000  0.444000  1.000000 0.075991
C9     1  0.740000  0.380000  0.496000  1.000000 0.075991
C10    1  0.610000  0.310000  0.523000  1.000000 0.075991
C11    1  0.400000  0.290000  0.497000  1.000000 0.075991
C12    1  0.330000  0.340000  0.446000  1.000000 0.075991
H1     2  0.520000  0.100000  0.170000  1.000000 0.091189
H2     2  0.750000  0.160000  0.149000  1.000000 0.091189
H3     2  0.840000  0.270000  0.590000  1.000000 0.091189
H4     2  0.610000  0.190000  0.585000  1.000000 0.091189
H5     2  0.120000  0.300000  0.301000  1.000000 0.091189
H6     2  0.220000  0.180000  0.224000  1.000000 0.091189
H7     2  0.840000  0.310000  0.194000  1.000000 0.091189
H8     2  0.750000  0.440000  0.273000  1.000000 0.091189
H9     2  0.780000  0.480000  0.422000  1.000000 0.091189
H10    2  0.900000  0.400000  0.516000  1.000000 0.091189
H11    2  0.300000  0.230000  0.518000  1.000000 0.091189
H12    2  0.170000  0.320000  0.426000  1.000000 0.091189
N1     3  0.590000  0.170000  0.161000  1.000000 0.075991
N2     3  0.690000  0.250000  0.573000  1.000000 0.075991
O1     4  0.510000  0.550000  0.339000  1.000000 0.075991
O2     4  0.140000  0.480000  0.352000  1.000000 0.075991
S1     5  0.380000  0.460000  0.350000  1.000000 0.075991
C13    1  0.620000 -0.030000  0.396000  0.780000 0.075991
C14    1  0.810000 -0.010000  0.440000  0.780000 0.075991
C15    1  0.980000  0.050000  0.411000  0.780000 0.075991
C16    1  0.890000  0.150000  0.385000  0.780000 0.075991
C17    1  0.700000  0.120000  0.338000  0.780000 0.075991
C18    1  0.520000  0.060000  0.363000  0.780000 0.075991
H13    2  0.740000  0.020000  0.480000  0.780000 0.091189
H14    2  0.870000 -0.080000  0.456000  0.780000 0.091189
H15    2  1.110000  0.070000  0.446000  0.780000 0.091189
H16    2  1.070000  0.010000  0.375000  0.780000 0.091189
H17    2  1.020000  0.190000  0.363000  0.780000 0.091189
H18    2  0.820000  0.190000  0.423000  0.780000 0.091189
H19    2  0.770000  0.090000  0.296000  0.780000 0.091189
H20    2  0.630000  0.190000  0.323000  0.780000 0.091189
H21    2  0.430000  0.100000  0.399000  0.780000 0.091189
H22    2  0.410000  0.030000  0.327000  0.780000 0.091189
O3     4  0.540000 -0.110000  0.386000  0.780000 0.075991
C13b   1  0.890000  0.030000  0.375000  0.220000 0.075991
C14b   1  1.010000  0.100000  0.334000  0.220000 0.075991
C15b   1  0.850000  0.180000  0.312000  0.220000 0.075991
C16b   1  0.740000  0.230000  0.366000  0.220000 0.075991
C17b   1  0.610000  0.160000  0.405000  0.220000 0.075991
C18b   1  0.760000  0.080000  0.427000  0.220000 0.075991
H13b   2  1.140000  0.140000  0.362000  0.220000 0.091189
H14b   2  1.090000  0.060000  0.296000  0.220000 0.091189
H15b   2  0.950000  0.240000  0.285000  0.220000 0.091189
H16b   2  0.730000  0.150000  0.280000  0.220000 0.091189
H17b   2  0.630000  0.290000  0.348000  0.220000 0.091189
H18b   2  0.860000  0.270000  0.395000  0.220000 0.091189
H19b   2  0.470000  0.130000  0.377000  0.220000 0.091189
H20b   2  0.540000  0.200000  0.445000  0.220000 0.091189
H21b   2  0.880000  0.100000  0.461000  0.220000 0.091189
H22b   2  0.660000  0.020000  0.450000  0.220000 0.091189
O3b    4  0.900000 -0.060000  0.367000  0.220000 0.075991
END
```

3.4.4. Dimethyl Formamide Solvate

```
TITL S-DMF
CELL 0.71073 6.10235 12.6884 21.323 90 92.2079 90
ZERR 4 0.00015 0.0004 0.0005 0 0.0011 0
LATT 1
SYMM 1/2-x,1/2+y,1/2-z
SFAC C H N O S
UNIT 72 104 16 16 4
FVAR 1.00
C1     1  0.340000  0.180000  0.059000  1.000000 0.079284
C2     1  0.420000  0.240000  0.013000  1.000000 0.079284
C3     1  0.630000  0.220000 -0.012000  1.000000 0.079284
C4     1  0.750000  0.140000  0.012000  1.000000 0.079284
C5     1  0.670000  0.070000  0.058000  1.000000 0.079284
C6     1  0.470000  0.090000  0.083000  1.000000 0.079284
C7     1  0.430000  0.100000  0.213000  1.000000 0.079284
C8     1  0.660000  0.090000  0.241000  1.000000 0.079284
C9     1  0.700000  0.160000  0.292000  1.000000 0.079284
C10    1  0.550000  0.230000  0.313000  1.000000 0.079284
C11    1  0.340000  0.230000  0.283000  1.000000 0.079284
C12    1  0.290000  0.160000  0.233000  1.000000 0.079284
H1     2  0.650000  0.360000 -0.070000  1.000000 0.095242
H2     2  0.870000  0.270000 -0.074000  1.000000 0.095242
H3     2  0.750000  0.310000  0.373000  1.000000 0.095242
H4     2  0.500000  0.360000  0.364000  1.000000 0.095242
H5     2  0.180000  0.200000  0.077000  1.000000 0.095242
H6     2  0.330000  0.310000 -0.005000  1.000000 0.095242
H7     2  0.910000  0.120000 -0.008000  1.000000 0.095242
H8     2  0.770000  0.010000  0.077000  1.000000 0.095242
H9     2  0.780000  0.040000  0.224000  1.000000 0.095242
H10    2  0.840000  0.160000  0.320000  1.000000 0.095242
H11    2  0.210000  0.280000  0.300000  1.000000 0.095242
H12    2  0.130000  0.160000  0.210000  1.000000 0.095242
N1     3  0.720000  0.290000 -0.057000  1.000000 0.079284
N2     3  0.590000  0.290000  0.363000  1.000000 0.079284
O1     4  0.510000 -0.080000  0.152000  1.000000 0.079284
O2     4  0.140000  0.010000  0.138000  1.000000 0.079284
S1     5  0.370000  0.020000  0.145000  1.000000 0.079284
C13    1  0.530000  0.440000  0.138000  0.595000 0.079284
C14    1  0.860000  0.470000  0.080000  0.595000 0.079284
C15    1  0.860000  0.350000  0.169000  0.595000 0.079284
H13    2  0.470000  0.390000  0.177000  0.595000 0.095242
H14    2  0.750000  0.510000  0.047000  0.595000 0.095242
H15    2  0.980000  0.530000  0.100000  0.595000 0.095242
H16    2  0.960000  0.410000  0.054000  0.595000 0.095242
H17    2  1.010000  0.380000  0.190000  0.595000 0.095242
H18    2  0.910000  0.280000  0.141000  0.595000 0.095242
H19    2  0.760000  0.320000  0.207000  0.595000 0.095242
N3     3  0.750000  0.420000  0.129000  0.595000 0.079284
O3     4  0.420000  0.500000  0.107000  0.595000 0.079284
C13b   1  0.710000  0.500000  0.080000  0.405000 0.079284
C14b   1  0.600000  0.360000  0.149000  0.405000 0.079284
C15b   1  0.990000  0.390000  0.133000  0.405000 0.079284
H13b   2  0.850000  0.540000  0.060000  0.405000 0.095242
H14b   2  0.440000  0.380000  0.132000  0.405000 0.095242
H15b   2  0.610000  0.270000  0.137000  0.405000 0.095242
H16b   2  0.620000  0.370000  0.200000  0.405000 0.095242
H17b   2  1.030000  0.310000  0.126000  0.405000 0.095242
H18b   2  1.030000  0.410000  0.183000  0.405000 0.095242
H19b   2  1.100000  0.440000  0.103000  0.405000 0.095242
N3b    3  0.760000  0.420000  0.117000  0.405000 0.079284
O3b    4  0.520000  0.530000  0.069000  0.405000 0.079284
END
```

3.4.5. Methyl Ethyl Ketone Solvate

```
TITL S_MEK
CELL 0.71073 8.60845 16.3204 25.0267 90 90 90
ZERR 8 0.00014 0.0002 0.0005 0 0 0
LATT 1
SYMM -x,1/2+y,1/2-z
SYMM 1/2-x,-y,1/2+z
SYMM 1/2+x,1/2-y,-z
SFAC C H N O S
UNIT 160 224 16 32 8
FVAR 1.00
C1     1  0.170000  0.560000  0.137000  1.000000 0.075991
C2     1  0.170000  0.566000  0.079000  1.000000 0.075991
C3     1  0.310000  0.568000  0.053000  1.000000 0.075991
C4     1  0.450000  0.569000  0.083000  1.000000 0.075991
C5     1  0.440000  0.565000  0.139000  1.000000 0.075991
C6     1  0.300000  0.565000  0.165000  1.000000 0.075991
C7     1 -0.070000  0.460000  0.181000  1.000000 0.075991
C8     1 -0.180000  0.423000  0.148000  1.000000 0.075991
C9     1 -0.210000  0.341000  0.155000  1.000000 0.075991
C10    1 -0.140000  0.296000  0.197000  1.000000 0.075991
C11    1 -0.030000  0.337000  0.230000  1.000000 0.075991
C12    1  0.000000  0.419000  0.223000  1.000000 0.075991
H1     2  0.060000  0.566000  0.056000  1.000000 0.091189
H2     2  0.320000  0.569000  0.010000  1.000000 0.091189
H3     2  0.550000  0.564000  0.163000  1.000000 0.091189
H4     2  0.300000  0.564000  0.208000  1.000000 0.091189
H5     2 -0.240000  0.456000  0.115000  1.000000 0.091189
H6     2 -0.290000  0.310000  0.129000  1.000000 0.091189
H7     2  0.030000  0.303000  0.261000  1.000000 0.091189
H8     2  0.080000  0.450000  0.249000  1.000000 0.091189
H9     2  0.690000  0.587000  0.081000  1.000000 0.091189
H10    2  0.600000  0.593000  0.019000  1.000000 0.091189
H11    2 -0.110000  0.183000  0.234000  1.000000 0.091189
H12    2 -0.240000  0.184000  0.180000  1.000000 0.091189
N1     3  0.600000  0.568000  0.060000  1.000000 0.075991
N2     3 -0.170000  0.225000  0.207000  1.000000 0.075991
O1     4  0.010000  0.601000  0.222000  1.000000 0.075991
O2     4 -0.130000  0.600000  0.134000  1.000000 0.075991
S1     5 -0.010000  0.562000  0.170000  1.000000 0.075991
C1a    1 -0.280000  0.704000 -0.043000  0.229000 0.075991
C2a    1 -0.464000  0.687000 -0.122000  0.229000 0.075991
C3a    1 -0.441000  0.683000 -0.062000  0.229000 0.075991
C4a    1 -0.243000  0.682000  0.014000  0.229000 0.075991
H1a    2 -0.381000  0.647000 -0.143000  0.229000 0.091189
H2a    2 -0.449000  0.749000 -0.137000  0.229000 0.091189
H3a    2 -0.582000  0.666000 -0.133000  0.229000 0.091189
H4a    2 -0.520000  0.727000 -0.042000  0.229000 0.091189
H5a    2 -0.473000  0.623000 -0.046000  0.229000 0.091189
H6a    2 -0.221000  0.615000  0.016000  0.229000 0.091189
H7a    2 -0.342000  0.694000  0.040000  0.229000 0.091189
H8a    2 -0.140000  0.714000  0.028000  0.229000 0.091189
O3a    4 -0.182000  0.738000 -0.072000  0.229000 0.075991
C1b    1 -0.274000  0.669100 -0.084600  0.771000 0.075991
C2b    1 -0.066000  0.671700 -0.011400  0.771000 0.075991
C3b    1 -0.105000  0.679100 -0.070400  0.771000 0.075991
C4b    1 -0.320000  0.696400 -0.139400  0.771000 0.075991
H1b    2 -0.134000  0.715300  0.012800  0.771000 0.091189
H2b    2 -0.092000  0.609900  0.003400  0.771000 0.091189
H3b    2  0.057000  0.684300 -0.004500  0.771000 0.091189
H4b    2 -0.042000  0.632100 -0.093900  0.771000 0.091189
H5b    2 -0.064000  0.737600 -0.087200  0.771000 0.091189
H6b    2 -0.327000  0.763800 -0.139700  0.771000 0.091189
H7b    2 -0.233000  0.679500 -0.169300  0.771000 0.091189
H8b    2 -0.433000  0.671000 -0.150100  0.771000 0.091189
O3b    4 -0.370000  0.640500 -0.053000  0.771000 0.075991
END
```

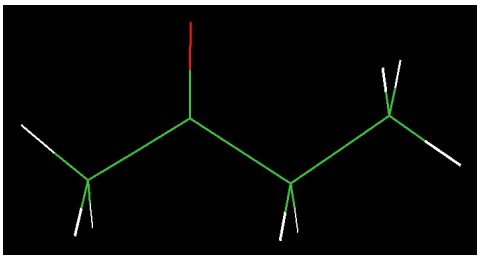
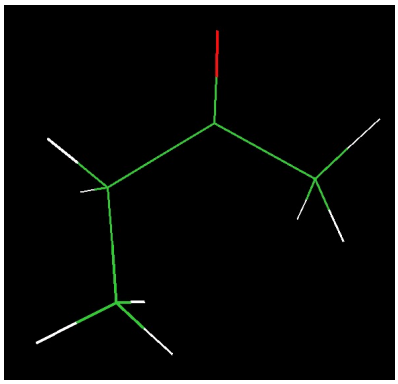
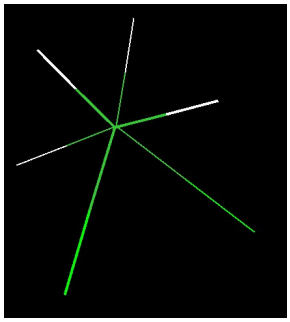
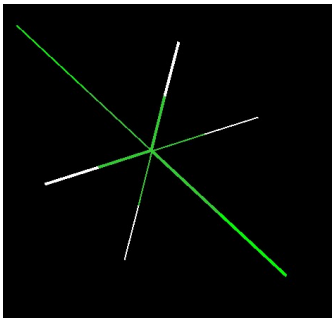
3.4.6. 1,2-Dichloroethane Solvate

```
TITL S-DCE
CELL 0.71073 8.67556 16.758 23.1266 90 90 90
ZERR 8 0.00018 0.0003 0.0005 0 0 0
LATT 1
SYMM -x,1/2+y,1/2-z
SYMM 1/2-x,-y,1/2+z
SYMM 1/2+x,1/2-y,-z
SFAC C H N O S Cl
UNIT 128 160 16 16 8 32
FVAR 1.00
C1     1  1.008000  0.050000  0.226000  1.000000 0.075991
C2     1  1.043000 -0.029000  0.236000  1.000000 0.075991
C3     1  1.151000 -0.070000  0.201000  1.000000 0.075991
C4     1  1.224000 -0.027000  0.156000  1.000000 0.075991
C5     1  1.190000  0.053000  0.146000  1.000000 0.075991
C6     1  1.080000  0.092000  0.180000  1.000000 0.075991
C7     1  0.845000  0.187000  0.131000  1.000000 0.075991
C8     1  0.834000  0.172000  0.069000  1.000000 0.075991
C9     1  0.692000  0.176000  0.042000  1.000000 0.075991
C10    1  0.557000  0.192000  0.074000  1.000000 0.075991
C11    1  0.570000  0.202000  0.134000  1.000000 0.075991
C12    1  0.712000  0.199000  0.161000  1.000000 0.075991
H1     2  1.121000 -0.181000  0.240000  1.000000 0.091189
H2     2  1.255000 -0.179000  0.183000  1.000000 0.091189
H3     2  0.403000  0.184000  0.005000  1.000000 0.091189
H4     2  0.320000  0.208000  0.071000  1.000000 0.091189
H5     2  0.924000  0.080000  0.253000  1.000000 0.091189
H6     2  0.987000 -0.061000  0.271000  1.000000 0.091189
H7     2  1.310000 -0.056000  0.129000  1.000000 0.091189
H8     2  1.248000  0.085000  0.112000  1.000000 0.091189
H9     2  0.937000  0.161000  0.043000  1.000000 0.091189
H10    2  0.684000  0.166000 -0.005000  1.000000 0.091189
H11    2  0.467000  0.213000  0.160000  1.000000 0.091189
H12    2  0.719000  0.208000  0.208000  1.000000 0.091189
N1     3  1.184000 -0.148000  0.211000  1.000000 0.075991
N2     3  0.418000  0.202000  0.047000  1.000000 0.075991
O1     4  1.139000  0.223000  0.125000  1.000000 0.075991
O2     4  1.004000  0.231000  0.220000  1.000000 0.075991
S1     5  1.026000  0.190000  0.165000  1.000000 0.075991
C13    1  0.660000  0.418000  0.104000  0.574000 0.075991
C14    1  0.790000  0.479000  0.107000  0.574000 0.075991
H13    2  0.570000  0.439000  0.130000  0.574000 0.091189
H14    2  0.700000  0.360000  0.120000  0.574000 0.091189
H15    2  0.830000  0.485000  0.152000  0.574000 0.091189
H16    2  0.760000  0.537000  0.090000  0.574000 0.091189
Cl1    6  0.590000  0.405000  0.032000  0.574000 0.136784
Cl2    6  0.960000  0.447000  0.067000  0.574000 0.136784
C13b   1  0.637000  0.423000  0.083000  0.426000 0.075991
C14b   1  0.765000  0.440000  0.125000  0.426000 0.075991
H13b   2  0.535000  0.458000  0.095000  0.426000 0.091189
H14b   2  0.606000  0.359000  0.083000  0.426000 0.091189
H15b   2  0.728000  0.423000  0.169000  0.426000 0.091189
H16b   2  0.799000  0.502000  0.125000  0.426000 0.091189
Cl1b   6  0.687000  0.449000  0.011000  0.426000 0.136784
Cl2b   6  0.933000  0.382000  0.109000  0.426000 0.136784
END
```

4. Computationally Generated Monosolvate Structures

4.1. Solvent Molecule Conformations

Each two low energy solvent molecule conformations were used as input for the rigid body **SMEK** and **SDCE** CSP searches.

Methyl ethyl ketone		
ΔE_{intra} / kJ mol^{-1}	0	7.40
1,2-Dichloroethane		
ΔE_{intra} / kJ mol^{-1}	5.97	0

4.2. 0 K Crystal Energy Landscapes

Table S9. Hypothetical low-energy crystal structures of **DDS Carbon Tetrachloride Monosolvate**. Isostructural S_{CTC} packings (solvent class M1) differing in solvent molecule orientations are highlighted in colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
1169	$P2_1$	5.687	17.594	8.687	90	104.32	90	–164.52	3.85	–237.20	0	–230.69	0	69.8	M1
108	$P2_1$	5.951	13.346	11.315	90	103.49	90	–168.38	0	–233.36	3.84	–229.26	1.43	67.1	
188	$P2_1$	5.766	17.756	8.581	90	104.17	90	–163.30	5.07	–234.76	2.44	–228.48	2.21	68.8	M1
9172	$P2_1$	5.788	17.685	8.574	90	104.04	90	–160.98	7.39	–234.23	2.97	–228.41	2.27	68.9	M1
280	*Ia*	16.85	6.001	17.632	90	101.08	90	–164.91	3.47	–231.54	5.65	–226.98	3.71	66.8	
750	*P*1	5.922	8.482	9.085	81.16	89.64	75.55	–163.66	4.71	–228.24	8.96	–226.5	4.18	67.2	
653	$P2_1/c$	9.143	17.685	11.546	90	113.2	90	–160.57	7.81	–231.75	5.45	–226.5	4.19	68.4	
273	*Ia*	16.771	6.029	17.741	90	101.4	90	–165.83	2.55	–231.09	6.11	–226.29	4.39	66.5	
360	$P2_1/c$	9.182	17.625	11.525	90	113.38	90	–161.88	6.5	–230.62	6.58	–226.24	4.45	68.5	
395	$P2_1/c$	9.107	17.779	11.587	90	113.08	90	–159.70	8.67	–230.63	6.57	–225.91	4.78	68	
1397	$P2_1/n$	5.812	7.809	37.24	90	90.88	90	–166.62	1.76	–233.06	4.14	–225.8	4.88	69.4	
6447	$P2_12_12_1$	5.792	7.801	37.568	90	90	90	–165.15	3.23	–232.11	5.09	–225.22	5.47	69	
400	$P2_1/c$	9.199	17.655	11.563	90	112.79	90	–160.98	7.39	–229.47	7.73	–224.67	6.02	67.8	
697	*P*1	5.907	8.957	9.044	77.62	83.54	71.6	–163.45	4.93	–227.41	9.79	–224.45	6.24	66.1	
716	*P*1	5.917	8.910	9.074	76.89	83.7	71.79	–164.29	4.08	–227.30	9.9	–224.34	6.35	66.2	
298	$P2_1$	5.812	17.511	8.569	90	102.95	90	–163.17	5.2	–229.79	7.41	–224.24	6.44	69	M1
1317	$P2_1$	5.808	17.552	8.566	90	103.19	90	–162.45	5.93	–229.64	7.56	–224.11	6.58	69	M1
6566	*P*1	5.937	8.930	9.053	77.33	82.46	71.88	–165.70	2.68	–227.59	9.61	–224.04	6.65	66	
2184	$P2_1/n$	5.720	13.900	21.873	90	92.84	90	–162.56	5.82	–230.29	6.91	–223.64	7.04	67.4	
345	$P2_1/c$	9.075	17.753	11.492	90	111	90	–159.76	8.62	–228.38	8.82	–222.9	7.79	67.9	
5871	$P2_1$	5.806	7.788	19.116	90	97.93	90	–166.37	2.01	–230.49	6.71	–222.84	7.85	68.4	
4227	$P2_1/n$	5.687	13.994	21.86	90	93.3	90	–165.33	3.05	–229.12	8.08	–222.65	8.04	67.5	
72	$P2_1$	5.773	17.824	8.656	90	105.26	90	–160.45	7.93	–229.01	8.19	–222.54	8.14	68.3	M1
367	$P2_1/c$	9.055	17.817	11.475	90	111.04	90	–160.28	8.1	–227.73	9.47	–222.53	8.16	67.9	
851	$P2_1/c$	9.044	17.802	11.489	90	111.16	90	–160.20	8.18	–227.64	9.55	–222.32	8.36	68	
2977	$P2_1/n$	5.697	14.075	21.692	90	93.41	90	–162.78	5.6	–228.62	8.58	–221.82	8.87	67.5	
6179	$Pna2_1$	37.964	5.843	7.721	90	90	90	–165.15	3.23	–229.40	7.8	–221.55	9.13	68.5	
3306	*Cc*	5.895	21.959	13.753	90	93.12	90	–163.17	5.2	–222.84	14.36	–221.04	9.65	66	
3107	*Cc*	5.888	21.926	13.811	90	93.72	90	–164.06	4.32	–222.41	14.79	–220.95	9.73	66	
9887	$Pna2_1$	23.375	5.792	13.013	90	90	90	–163.12	5.26	–224.92	12.28	–220.55	10.14	66.5	
1144	$P2_12_12_1$	5.753	7.879	37.503	90	90	90	–167.51	0.87	–228.63	8.57	–220.5	10.19	69.2	
9866	$Pna2_1$	23.267	5.783	13.093	90	90	90	–164.11	4.27	–224.18	13.02	–219.7	10.99	66.6	
2691	$Pna2_1$	23.574	5.766	12.971	90	90	90	–163.26	5.12	–223.67	13.53	–219.37	11.31	66.6	

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
1063	$P2_1/n$	5.772	7.915	37.484	90	92.34	90	–163.64	4.74	–225.63	11.56	–218.01	12.68	68.7	
7242	$P2_1/n$	5.825	14.047	21.608	90	91.49	90	–163.84	4.54	–223.81	13.39	–215.97	14.72	66.2	
2586	$P2_1/n$	5.795	14.191	21.452	90	91.08	90	–162.78	5.6	–222.82	14.37	–215.11	15.57	66.4	

[a]Rank CrystalPredictor; [b]calculated using Platon[2].

Table S10. Hypothetical low-energy crystal structures of **DDS Acetone Monosolvate**. Isostructural **S$_{ACO}$** (M2) and **S$_{DCE}$** (M7) packings differing in solvent molecule orientations are highlighted in colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
110	$P2_1/n$	5.914	12.012	21.650	90	93.16	90	–188.73	0.00	–267.71	0.00	–256.48	0.22	70.9	M2
653	$P2_1/c$	18.637	5.670	15.435	90	112.29	90	–179.39	9.34	–265.96	1.74	–256.70	0.00	72.4	
1590	$P2_1/n$	5.770	12.538	21.520	90	90.76	90	–187.59	1.15	–264.81	2.90	–254.40	2.30	69.9	M2
144	$P2_1/c$	17.850	5.713	15.603	90	100.38	90	–183.44	5.30	–260.79	6.92	–251.69	5.01	69.6	
2	$P2_1/n$	5.963	7.895	31.974	90	93.12	90	–181.07	7.66	–259.49	8.22	–250.09	6.61	72.8	
2719	$P2_1$	5.920	7.993	16.094	90	96.77	90	–181.35	7.38	–259.37	8.33	–250.56	6.14	72.2	
5739	$P2_1/c$	17.719	5.534	15.787	90	97.18	90	–181.27	7.46	–259.36	8.35	–250.88	5.82	70.9	
57	$P2_1/c$	18.884	5.868	15.511	90	113.05	90	–179.18	9.55	–258.01	9.70	–249.57	7.14	68.9	
176	$P2_1$	5.982	8.016	16.234	90	97.86	90	–177.64	11.09	–257.26	10.44	–251.34	5.37	70.7	
82	$Pna2_1$	33.191	5.946	7.777	90	90	90	–179.46	9.27	–256.09	11.62	–248.24	8.46	71.0	
495	$P2_12_12_1$	5.935	7.797	32.991	90	90	90	–179.16	9.57	–255.35	12.36	–246.97	9.73	71.4	
756	$Pbca$	8.545	16.073	23.828	90	90	90	–176.25	12.48	–254.04	13.67	–246.65	10.05	66.2	M4
796	$Pbca$	8.536	16.023	23.937	90	90	90	–177.08	11.65	–253.74	13.97	–245.89	10.81	66.1	M4
128	$P2_1/c$	17.774	5.693	15.647	90	98.13	90	–182.03	6.71	–253.55	14.15	–244.35	12.35	69.5	
797	$Pbca$	8.543	16.050	23.982	90	90	90	–176.82	11.92	–253.53	14.17	–245.71	10.99	65.9	M4
1390	$Pbca$	9.039	15.903	22.279	90	90	90	–169.55	19.18	–246.22	21.48	–238.36	18.34	68.0	

[a]Rank CrystalPredictor; [b]calculated using Platon[2].

Table S11. Hypothetical low-energy crystal structures of **DDS Cyclohexanone Monosolvate**. Isostructural **SCHOX** (M2) and **SCTC** (M1) packings differing in solvent molecule orientations are highlighted in colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
17	$P2_1/n$	5.938	13.467	21.370	90	93.25	90	–199.24	2.37	–297.62	0.00	–281.61	0.00	72.8	M2
86	$P2_1/n$	6.090	12.926	21.701	90	90.41	90	–201.60	0.00	–296.56	1.06	–279.99	1.63	72.6	M2
5825	P-1	5.980	8.226	17.467	81.10	88.95	80.77	–195.02	6.58	–293.50	4.12	–277.56	4.06	74.4	
268	P-1	6.021	8.336	17.430	78.78	85.28	80.88	–193.38	8.22	–289.40	8.23	–275.20	6.41	73.9	
158	$Pna2_1$	21.510	6.415	12.863	90	90	90	–195.06	6.54	–287.31	10.31	–273.67	7.94	69.9	
353	$P2_1/n$	6.391	15.737	17.478	90	97.86	90	–192.99	8.62	–287.49	10.13	–273.11	8.50	71.5	
7154	$P2_1/c$	9.153	17.523	10.599	90	95.82	90	–195.30	6.31	–287.23	10.39	–272.28	9.33	73.9	
356	$P2_1/c$	17.585	6.090	16.273	90	100.25	90	–191.94	9.66	–287.83	9.79	–271.64	9.97	72.5	
105	$P2_1/n$	5.642	14.638	21.084	90	92.39	90	–199.88	1.73	–284.93	12.69	–270.06	11.55	71.6	M2
352	Cc	18.691	6.024	15.947	90	98.39	90	–192.34	9.26	–281.71	15.91	–269.82	11.79	69.9	
494	$Pna2_1$	15.712	6.146	18.365	90	90.00	90	–192.87	8.73	–281.48	16.14	–269.20	12.42	70.1	
63	$P2_1/n$	5.961	13.899	21.274	90	91.55	90	–194.38	7.22	–284.00	13.62	–269.06	12.55	70.5	M2
22	$P2_1$	6.056	12.972	11.390	90	101.93	90	–192.84	8.76	–282.73	14.89	–268.55	13.06	71.1	
72	$P2_1/n$	6.004	13.161	21.610	90	92.64	90	–192.58	9.02	–285.72	11.90	–268.42	13.19	73.1	M2
418	$P2_1/n$	5.872	14.520	21.041	90	92.32	90	–192.05	9.55	–277.98	19.64	–267.32	14.29	69.5	M2
1558	$P2_12_12_1$	10.991	11.542	13.709	90	90.00	90	–194.00	7.61	–280.26	17.36	–266.21	15.40	71.7	
794	$P2_12_12_1$	10.828	11.597	13.691	90	90.00	90	–193.95	7.65	–281.18	16.44	–265.34	16.27	72.6	
458	$P2_1$	6.425	17.699	7.951	90	102.88	90	–198.44	3.16	–279.18	18.44	–265.03	16.58	70.7	M1
3629	$P1$	6.084	8.325	8.970	83.76	86.44	73.92	–197.91	3.69	–280.03	17.59	–264.60	17.02	71.9	
219	$P2_1$	6.107	12.930	11.405	90	104.81	90	–191.92	9.68	–281.62	16.00	–264.41	17.20	71.5	
1642	$P2_1$	5.977	18.712	8.456	90	110.05	90	–192.16	9.44	–274.74	22.88	–263.42	18.19	70.1	M1
29	Pn	6.657	10.728	12.726	90	100.41	90	–193.35	8.26	–280.87	16.75	–263.27	18.34	69.4	
1075	$P2_1$	6.221	18.349	8.085	90	105.58	90	–191.31	10.29	–274.59	23.03	–262.44	19.17	70.1	M1
264	$P2_1$	6.180	18.235	8.385	90	108.08	90	–191.09	10.52	–270.13	27.49	–258.42	23.19	69.4	M1

[a]Rank CrystalPredictor; [b]calculated using Platon[2].

Table S12. Hypothetical low-energy crystal structures of **DDS Dimethylformamide Monosolvate**. Isostructural **S**$_{DMF}$ (M2) and **S**$_{CTC}$ (M1) packings differing in solvent molecule orientations are highlighted in colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
310	$P2_1/c$	17.5832	5.734	15.4364	90	98.88	90	–186.46	8.49	–285.26	0.00	–274.67	0.00	73.9	
29	$P2_1/c$	18.4942	5.8531	15.4435	90	111.22	90	–191.39	3.56	–283.42	1.85	–272.87	1.79	72.9	
21	$P2_1/n$	5.8388	12.0739	21.9341	90	92.391	90	–194.95	0.00	–285.22	0.04	–271.73	2.94	73.3	M2
45	$P2_1/n$	5.8502	12.02	21.9149	90	91.17	90	–191.75	3.20	–284.00	1.26	–271.61	3.06	73.6	M2
388	$P2_1/c$	18.5296	5.9461	15.3882	90	112.36	90	–190.27	4.68	–283.06	2.20	–271.23	3.44	72.6	
54	$P2_1/c$	17.7744	5.6482	15.6011	90	97.315	90	–193.17	1.78	–281.81	3.46	–269.29	5.38	73.2	
3	$P2_1/n$	5.8932	12.4737	21.4547	90	92.273	90	–193.78	1.17	–283.23	2.03	–267.88	6.78	72.0	M2
276	$P2_1/c$	18.2408	5.7406	15.5213	90	105.83	90	–186.20	8.75	–278.92	6.35	–267.60	7.07	72.7	
72	$Pbca$	5.8651	15.4747	35.0739	90	90	90	–187.67	7.28	–277.25	8.02	–267.20	7.46	71.4	
84	$Pbca$	5.7645	15.547	35.3875	90	90	90	–189.01	5.94	–276.31	8.96	–267.17	7.50	71.6	
2369	$P2_1/c$	17.6605	5.8508	15.4756	90	99.428	90	–191.26	3.69	–280.00	5.27	–266.97	7.70	71.9	
6906	$P2_12_12_1$	8.3269	10.5065	18.3255	90	90	90	–186.01	8.94	–278.45	6.81	–266.25	8.42	70.9	
164	$I2/a$	15.8618	5.7407	34.8662	90	95.919	90	–187.92	7.03	–275.26	10.01	–265.82	8.84	72.0	
62	$P2_1/c$	18.9701	5.9064	15.3378	90	111.85	90	–185.87	9.08	–274.58	10.68	–265.03	9.64	71.3	
279	$Pbca$	12.3078	11.737	22.9194	90	90	90	–181.59	13.36	–275.01	10.26	–264.39	10.27	68.2	
111	$P2_1/c$	17.9301	5.7928	15.4969	90	97.824	90	–188.02	6.93	–274.36	10.90	–264.13	10.54	72.1	
952	$P2_12_12_1$	5.9248	7.7899	34.0498	90	90	90	–188.13	6.82	–273.91	11.35	–262.99	11.67	72.3	
118	$P2_1$	5.9139	7.8059	17.4847	90	93.729	90	–186.13	8.82	–270.41	14.86	–262.16	12.50	70.6	M1
79	$P2_1/c$	5.9529	7.6811	34.8969	90	90.95	90	–188.48	6.47	–270.57	14.69	–261.01	13.66	71.3	
134	$P2_1/n$	5.677	13.5611	21.2607	90	92.619	90	–191.63	3.32	–272.27	12.99	–260.95	13.72	69.4	M2
198	$P2_1$	5.9555	7.7798	17.112	90	94.974	90	–187.22	7.73	–270.66	14.60	–260.76	13.91	72.1	M1
260	$Pbca$	8.4474	16.1799	24.9818	90	90	90	–182.60	12.35	–262.73	22.53	–254.98	19.69	66.5	
269	$Pbca$	8.4497	16.2401	24.8954	90	90	90	–182.95	12.00	–262.75	22.51	–254.96	19.71	66.5	

[a]Rank CrystalPredictor; [b]calculated using Platon[2].

Table S13. Hypothetical low-energy crystal structures of **DDS Tetrahydrofuran Monosolvate**. Isostructural **S**$_{THF}$ (M2) packings differing in solvent molecule orientations are highlighted in colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
80	$P2_1/c$	18.655	5.792	15.992	90	114.95	90	–184.57	10.16	–275.06	3.84	–264.54	0.00	72.7	
1941	$P2_1/n$	5.623	12.899	21.728	90	90.78	90	–194.72	0.00	–277.65	1.25	–264.53	0.01	72.2	M2
31	$P2_1/n$	5.868	12.232	21.870	90	92.38	90	–189.92	4.80	–278.90	0.00	–262.72	1.82	72.5	M2
367	$Pbca$	5.892	16.293	35.165	90	90	90	–183.66	11.06	–272.45	6.45	–262.24	2.30	67.8	
486	$P2_1/c$	17.347	5.679	16.081	90	99.00	90	–188.30	6.43	–272.97	5.93	–262.22	2.32	72.8	
53	$P2_1/n$	5.719	12.922	21.781	90	91.32	90	–189.60	5.13	–268.85	10.05	–259.86	4.68	70.9	M2
70	$P2_1/c$	18.364	5.983	15.412	90	112.57	90	–180.86	13.86	–274.25	4.65	–259.67	4.86	72.9	
1723	$P2_1/c$	17.676	5.746	16.048	90	99.80	90	–183.33	11.40	–266.30	12.60	–258.01	6.53	71.2	
101	$P2_1/c$	17.328	5.865	15.633	90	99.47	90	–183.86	10.86	–271.00	7.90	–257.28	7.25	72.7	
118	$P2_12_12_1$	5.853	7.791	34.677	90	90	90	–181.64	13.09	–265.20	13.70	–253.96	10.57	72.2	
134	$P2_1/n$	5.936	7.639	35.524	90	90.21	90	–179.77	14.96	–261.49	17.41	–250.28	14.26	70.8	
11	$P2_1/c$	5.792	12.689	11.461	90	104.08	90	–181.14	13.59	–258.40	20.50	–247.33	17.21	69.7	
19	Ic	16.201	5.881	17.695	90	100.79	90	–182.30	12.43	–256.73	22.17	–244.64	19.90	68.8	
37	Cc	5.724	22.651	12.668	90	95.60	90	–179.86	14.87	–255.66	23.25	–244.63	19.90	70	
14	Ia	16.184	5.773	17.943	90	98.93	90	–182.51	12.22	–254.37	24.53	–241.38	23.16	68.7	

[a]Rank CrystalPredictor; [b]calculated using Platon[2].

Table S14. Hypothetical low-energy crystal structures of **DDS Methyl Ethyl Ketone Monosolvate**. Isostructural **SMEK** (M3), **SACO** (M2), and **SDCE** (M4) packings differing in solvent molecule orientations are highlighted in light colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
62[1]	*Pbca*	8.795	15.726	24.303	90	90	90	–185.79	6.21	–273.47	0.00	–263.51	0.00	68.6	M3
91[1]	*P*2$_1$/*n*	5.564	13.375	21.992	90	90.39	90	–188.67	3.33	–271.10	2.37	–260.75	2.77	70.7	M2
64[1]	*P*2$_1$/*n*	5.561	13.385	22.045	90	90.24	90	–188.68	3.32	–270.68	2.79	–260.71	2.80	70.4	M2
9175[1]	*P*2$_1$/*n*	7.551	13.791	15.856	90	100.09	90	–185.43	6.57	–271.34	2.13	–259.36	4.15	70.8	
2184[1]	*P*2$_1$2$_1$2$_1$	6.461	10.511	23.966	90	90	90	–186.49	5.51	–270.60	2.87	–259.10	4.41	71.0	
2403[1]	*P*2$_1$2$_1$2$_1$	6.510	10.516	23.873	90	90	90	–186.92	5.08	–271.00	2.47	–258.91	4.60	70.7	
969[1]	*P*2$_1$/*n*	8.149	10.565	19.060	90	96.66	90	–183.98	8.02	–273.01	0.45	–258.46	5.05	70.7	
270[1]	*Pbca*	8.425	16.690	24.048	90	90	90	–183.51	8.49	–268.64	4.83	–258.21	5.30	68.2	M4
73[1]	*P*2$_1$/*c*	18.971	5.993	15.561	90	113.18	90	–182.49	9.51	–268.79	4.68	–258.14	5.38	71.1	
1278[1]	*P*2$_1$/*n*	5.778	13.318	21.553	90	91.46	90	–192.00	0.00	–269.67	3.80	–257.94	5.58	69.7	M2
106[1]	*P*2$_1$/*n*	5.723	13.094	21.695	90	90.06	90	–189.79	2.21	–267.61	5.86	–257.69	5.83	71.2	M2
206[1]	*P*2$_1$/*n*	7.689	13.658	15.999	90	100.87	90	–186.36	5.64	–269.56	3.91	–257.51	6.01	69.8	
1684[1]	*P*2$_1$/*c*	8.793	12.344	15.560	90	105.31	90	–182.39	9.61	–270.19	3.28	–257.45	6.06	71.0	
160[1]	*P*2$_1$/*c*	19.003	5.963	15.594	90	113.00	90	–182.39	9.61	–267.77	5.70	–257.09	6.43	71.1	
327[1]	*P*2$_1$/*n*	5.418	13.938	21.939	90	92.75	90	–184.46	7.54	–264.17	9.30	–256.46	7.05	69.6	
198[1]	*P*2$_1$/*n*	5.604	7.829	36.661	90	93.25	90	–185.55	6.45	–268.04	5.43	–256.37	7.14	72.2	
333[1]	*P*2$_1$/*c*	17.910	5.889	15.666	90	100.38	90	–184.64	7.36	–267.82	5.65	–256.37	7.15	71.1	
1094[1]	*Pbca*	8.520	15.519	25.597	90	90	90	–177.38	14.62	–267.80	5.67	–255.42	8.10	67.9	
464[1]	*P*2$_1$/*n*	5.647	7.804	36.628	90	93.28	90	–184.40	7.60	–267.40	6.07	–255.19	8.32	71.9	
681[1]	*P*2$_1$2$_1$2$_1$	5.568	7.845	36.800	90	90	90	–182.58	9.42	–268.54	4.93	–255.12	8.40	72.0	
590[1]	*P*2$_1$/*c*	18.495	5.702	15.879	90	100.82	90	–182.71	9.29	–264.81	8.66	–254.69	8.82	70.4	
436[1]	*Pbca*	8.509	15.418	25.415	90	90	90	–179.99	12.01	–265.91	7.56	–254.05	9.47	69.1	M4
133[1]	*P*2$_1$/*c*	18.258	5.862	15.694	90	101.61	90	–184.68	7.32	–264.32	9.15	–252.61	10.91	70.2	
112[1]	*P*2$_1$/*n*	5.585	13.494	22.261	90	91.25	90	–183.80	8.20	–261.05	12.42	–252.48	11.03	68.8	
1449[1]	*Pbca*	8.628	16.253	24.528	90	90	90	–173.46	18.54	–259.37	14.10	–251.15	12.36	67.0	
402[1]	*Pbca*	8.412	15.660	25.251	90	90	90	–176.86	15.14	–262.90	10.57	–251.15	12.37	69.4	M4
118[1]	*P*2$_1$/*c*	18.579	5.560	16.718	90	101.37	90	–183.85	8.15	–259.15	14.31	–251.01	12.50	68.1	
564[1]	*Pbca*	8.481	16.383	24.458	90	90	90	–178.31	13.69	–259.60	13.87	–250.10	13.42	68.0	M4
7688[1]	*P*2$_1$/*c*	12.446	7.750	17.446	90	91.68	90	–183.84	8.16	–258.92	14.55	–249.27	14.24	68.7	
860[1]	*P*2$_1$/*c*	12.512	7.716	17.434	90	92.03	90	–183.24	8.76	–258.86	14.60	–249.19	14.32	68.7	
136[1]	*P*2$_1$	5.856	7.699	18.301	90	98.28	90	–180.20	11.80	–258.56	14.91	–246.42	17.10	70.9	
371[2]	*P*2$_1$/*n*	6.023	12.952	21.179	90	95.14	90	–182.77	9.23	–267.35	6.12	–255.05	5.70	70.1	M2
40[2]	*P*2$_1$/*n*	5.637	13.655	21.527	90	91.28	90	–183.54	8.46	–262.39	11.08	–250.69	10.05	69.9	M2

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
24^2	$P2_1/n$	5.536	13.602	21.909	90	90.63	90	–184.67	7.33	–260.22	13.25	–248.96	11.78	70.2	M2
120^2	$Pbca$	8.435	16.677	24.395	90	90	90	–171.49	20.51	–253.74	19.73	–244.66	16.09	67.3	

[a]Rank CrystalPredictor, superscript 1 and 2 indicate the two different conformations used as input for the searches; [b]calculated using Platon[2].

Table S15. Hypothetical low-energy crystal structures of **DDS Dichloroethane Monosolvate**. Isostructural **S$_{DCE}$** (M4) and **S$_{ACO}$** (M2) packings differing in solvent molecule orientations are highlighted in colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
713^1	$Pbca$	8.684	16.305	23.278	90	90	90	–174.66	7.35	–245.36	4.54	–241.77	0.00	68.1	M4
1490^1	$Pbca$	8.646	16.642	22.816	90	90	90	–172.30	9.70	–247.02	2.88	–240.98	0.80	68.6	M4
6^2	$P2_1$	5.779	13.153	11.222	90	104.56	90	–181.11	0.90	–241.42	8.47	–240.38	1.40	68.2	
46^2	$P2_12_12_1$	5.732	7.705	35.389	90	90	90	–182.01	0.00	–249.90	0.00	–240.29	1.48	72.4	
250^2	$Pna2_1$	35.199	5.733	7.771	90	90	90	–178.05	3.96	–247.90	1.99	–239.73	2.04	72.0	
334^2	$Pna2_1$	34.794	5.756	7.840	90	90	90	–175.99	6.02	–247.51	2.39	–239.25	2.52	72.0	
67^2	$P2_12_12_1$	5.753	7.858	34.885	90	90	90	–178.31	3.70	–246.55	3.35	–238.88	2.90	71.6	
232^1	$P2_1/c$	17.730	5.765	15.809	90	98.41	90	–176.15	5.85	–245.95	3.95	–238.19	3.59	70.7	
23^1	$P2_1/n$	5.736	12.648	22.117	90	90.14	90	–176.32	5.68	–245.09	4.81	–237.33	4.44	70.4	M2
284^2	$P2_1$	5.983	7.850	17.286	90	99.16	90	–174.81	7.20	–244.70	5.20	–236.87	4.90	70.5	
121^2	$P2_12_12_1$	5.528	8.033	35.106	90	90	90	–179.08	2.93	–245.08	4.82	–236.87	4.91	72.5	
138^2	$P2_1/n$	5.733	7.755	35.458	90	92.08	90	–174.91	7.10	–245.21	4.69	–236.81	4.97	71.8	
3462^1	$P2_1/n$	5.686	12.931	22.064	90	90.18	90	–172.62	9.39	–243.06	6.84	–236.39	5.38	69.4	M2
118^2	$P2_1/n$	5.841	7.899	34.267	90	93.27	90	–174.38	7.62	–243.72	6.18	–236.14	5.63	71.6	
432^1	P21/c	5.488	7.957	35.811	90	91.64	90	–175.76	6.25	–244.73	5.17	–236.13	5.64	72.3	
41^2	$P2_1$	5.678	13.238	11.247	90	104.26	90	–179.18	2.82	–244.69	5.21	–235.92	5.85	68.6	
191^1	$P2_1/n$	5.561	12.876	22.305	90	91.56	90	–175.91	6.10	–245.50	4.40	–235.60	6.18	70.6	M2
33^2	Ic	15.691	5.954	18.051	90	96.19	90	–178.52	3.49	–241.83	8.06	–235.00	6.77	67.0	
335^1	$P2_1$	5.869	7.953	17.196	90	92.34	90	–173.12	8.89	–242.85	7.05	–234.94	6.83	70.4	
53^2	$P2_1$	5.939	12.627	11.546	90	104.28	90	–178.66	3.35	–243.10	6.79	–234.78	6.99	67.0	
342^1	$P2_1$	5.974	7.860	17.381	90	97.18	90	–173.25	8.76	–240.44	9.46	–234.77	7.00	69.7	
387^2	Pna21	34.808	5.908	7.818	90	90	90	–173.66	8.35	–242.42	7.48	–234.76	7.01	70.2	
76^2	Ic	16.693	5.766	17.421	90	98.00	90	–177.90	4.11	–241.81	8.08	–234.65	7.12	67.7	

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
840^2	$Pna2_1$	36.524	5.586	7.728	90	90	90	–176.45	5.56	–243.62	6.28	–234.63	7.14	71.7	
83^2	$P2_1$	5.634	13.076	11.537	90	103.44	90	–179.15	2.86	–241.42	8.47	–234.27	7.50	68.0	
436^1	$P2_1$	5.538	7.717	18.360	90	92.15	90	–174.10	7.91	–242.60	7.29	–234.10	7.68	72.2	
668^1	$P2_1$	5.925	7.746	17.813	90	99.42	90	–173.66	8.35	–240.87	9.03	–233.54	8.23	70.0	
487^2	$P2_1/n$	6.001	7.860	34.300	90	91.71	90	–173.47	8.53	–240.93	8.96	–232.83	8.94	69.8	
306^2	$P2_1$	5.922	7.741	17.817	90	98.52	90	–173.19	8.82	–240.99	8.90	–232.53	9.24	69.7	
850^2	$P2_1/n$	5.853	12.942	21.501	90	90.77	90	–173.34	8.67	–242.25	7.65	–232.51	9.26	69.0	M2
25^1	$P1$	5.618	8.429	9.196	98.28	91.84	105.28	–175.14	6.87	–239.36	10.53	–232.39	9.38	68.0	
2^1	$P2_1$	5.813	12.577	11.565	90	102.45	90	–178.60	3.40	–243.39	6.50	–232.26	9.51	68.1	
11^2	Ic	16.229	5.703	18.204	90	99.24	90	–178.71	3.29	–239.51	10.38	–231.84	9.94	67.8	
669^2	$P2_1$	8.779	10.249	9.284	90	106.29	90	–173.93	8.08	–239.07	10.82	–231.33	10.45	70.2	
222^2	$P2_12_12_1$	5.588	7.722	36.849	90	90	90	–174.92	7.09	–240.79	9.10	–231.16	10.61	71.1	
8^1	$P2_1$	5.736	12.794	11.619	90	99.90	90	–178.42	3.59	–238.32	11.58	–231.08	10.69	67.0	
114^2	Cc	5.747	22.515	13.011	90	92.75	90	–175.73	6.28	–235.31	14.59	–229.36	12.41	67.0	
207^2	$P1$	5.510	8.379	9.286	98.57	94.06	104.90	–173.54	8.47	–236.49	13.41	–229.29	12.49	69.2	
879^1	$P2_1$	5.655	13.093	11.435	90	101.35	90	–172.46	9.54	–237.09	12.81	–229.00	12.77	67.7	
157^2	$Pbca$	8.058	16.269	25.085	90	90	90	–167.40	14.61	–238.78	11.12	–227.61	14.16	68.4	
10^1	Cc	16.285	5.671	18.106	90	97.45	90	–178.25	3.76	–235.41	14.49	–226.88	14.90	67.9	

[a]Rank CrystalPredictor, superscript 1 and 2 indicate the two different conformations used as input for the searches; [b]calculated using Platon[2].

Table S16. Selected hypothetical low-energy crystal structures of **DDS 1,4-Dioxane Monosolvate**. Isostructural **SDX** (M5), **SCTC** (M1) and **SACO** (M2) packings differing in solvent molecule orientations are highlighted in colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/%[b]	
8676	$P2_1/n$	5.719	12.983	22.113	90	90.16	90	–189.74	0.00	–273.78	3.27	–262.74	0.00	71.4	M2
586	$Pbca$	11.806	11.399	24.424	90	90	90	–188.29	1.45	–277.05	0.00	–262.63	0.10	71	M5
207	$Pbca$	10.895	11.252	26.829	90	90	90	–187.73	2.01	–276.45	0.60	–262.10	0.63	71.3	M5
992	$P2_1/n$	5.728	12.946	22.129	90	90.48	90	–183.82	5.92	–272.36	4.70	–261.89	0.85	71.2	M2
8813	$P2_1/n$	5.666	12.680	22.401	90	90.03	90	–187.73	2.01	–272.41	4.64	–261.29	1.44	72.7	M2
498	$Pbca$	10.973	11.287	26.911	90	90	90	–185.16	4.58	–273.55	3.50	–259.15	3.58	70.2	M5
136	$P2_1/n$	5.778	22.620	12.491	90	96.76	90	–186.36	3.38	–270.60	6.45	–258.42	4.32	72.4	
158	$P2_1$	6.085	12.436	11.575	90	104.14	90	–183.82	5.92	–267.88	9.17	–257.53	5.21	68.9	
87	$P2_1/n$	5.779	7.806	35.941	90	91.97	90	–188.04	1.70	–269.11	7.94	–256.07	6.66	72.5	
140	$P2_1/c$	5.817	7.931	34.856	90	92.51	90	–186.11	3.63	–269.70	7.35	–256.04	6.69	73.3	
280	$P2_1/n$	5.779	22.619	12.347	90	97.37	90	–184.28	5.47	–271.24	5.81	–255.71	7.03	73.4	
228	$P2_1/c$	5.711	8.013	35.423	90	91.69	90	–185.18	4.57	–266.51	10.54	–255.67	7.06	72.6	
539	Cc	18.391	5.756	15.814	90	94.01	90	–180.17	9.58	–265.79	11.26	–254.98	7.76	69.9	
1094	$P2_1/n$	5.858	22.777	12.576	90	100.20	90	–184.81	4.93	–267.79	9.26	–254.54	8.20	71	
364	$Pbca$	8.693	16.308	23.760	90	90	90	–180.47	9.27	–267.86	9.19	–254.43	8.31	69.4	
77	$P2_12_12_1$	5.890	7.795	35.350	90	90	90	–187.17	2.57	–267.54	9.51	–254.19	8.55	72.4	
2551	$P2_1$	5.734	7.839	18.283	90	98.24	90	–185.72	4.03	–268.54	8.51	–254.15	8.59	72.3	
2264	$P2_12_12_1$	5.937	7.820	35.205	90	90	90	–189.95	-0.21	–266.88	10.17	–253.33	9.41	71.9	
396	$P2_1/c$	17.031	11.999	7.925	90	91.73	90	–180.87	8.87	–267.70	9.35	–252.84	9.90	72.6	
112	$P2_1/c$	5.868	7.779	35.954	90	92.50	90	–189.16	0.58	–266.29	10.76	–252.66	10.08	71.5	
72	$P2_1$	6.024	12.620	11.485	90	103.91	90	–184.38	5.36	–263.86	13.19	–252.05	10.69	69.2	
429	$Pna2_1$	37.445	5.687	7.775	90	90	90	–183.83	5.92	–264.07	12.98	–251.67	11.07	71.1	
22	Ia	16.096	5.813	18.035	90	97.61	90	–186.16	3.59	–264.46	12.59	–251.65	11.08	70	
340	$Pna2_1$	15.896	5.925	18.012	90	90	90	–183.46	6.29	–261.89	15.16	–251.20	11.53	69.1	
464	$P2_1/c$	17.687	11.723	7.986	90	101.22	90	–181.69	8.05	–264.14	12.91	–250.67	12.07	69.4	
680	$P2_1/c$	17.383	11.993	7.834	90	90.51	90	–180.14	9.60	–264.09	12.96	–250.52	12.22	72	
4625	$P2_1/c$	18.145	11.593	7.905	90	102.33	90	–181.36	8.38	–261.99	15.06	–250.28	12.45	72.4	
89	Ia	16.144	5.866	18.142	90	100.66	90	–180.42	9.32	–259.91	17.14	–250.01	12.73	69.4	
119	$P2_1$	5.765	13.097	11.421	90	103.78	90	–183.29	6.45	–261.88	15.17	–249.90	12.84	70.1	
378	$P2_1$	5.673	7.826	18.776	90	95.29	90	–183.10	6.64	–261.19	15.87	–248.49	14.24	70.8	
208	$P2_1$	5.859	17.906	8.366	90	104.31	90	–180.98	8.76	–257.54	19.51	–248.37	14.36	69.2	M1
135	$Pca2_1$	23.780	6.067	11.843	90	90	90	–184.13	5.61	–259.55	17.50	–248.30	14.44	68.5	
1	Ia	16.129	5.754	18.417	90	101.75	90	–186.82	2.93	–261.20	15.85	–247.99	14.75	70.1	

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}							
2631	$P2_1$	6.208	12.041	11.539	90	100.22	90	–180.67	9.07	–261.34	15.71	–247.81	14.93	69	
27	$P2_12_12_1$	6.580	7.192	34.534	90	90	90	–182.66	7.09	–261.55	15.50	–246.95	15.78	71.8	
253	$Pna2_1$	37.249	5.758	7.797	90	90	90	–182.76	6.98	–258.39	18.66	–246.95	15.79	70.2	
1062	$P1$	5.913	8.445	8.931	82.56	87.51	74.23	–181.69	8.06	–255.31	21.74	–245.61	17.13	68.9	
840	Cc	5.882	22.966	12.629	90	92.12	90	–181.02	8.72	–254.56	22.49	–245.20	17.54	68.9	
728	Ic	15.717	6.080	18.011	90	98.84	90	–183.59	6.15	–257.22	19.83	–245.10	17.63	68.8	
406	Cc	5.901	22.716	12.685	90	91.55	90	–182.24	7.51	–254.91	22.14	–243.39	19.34	69.1	

[a]Rank CrystalPredictor; [b]calculated using Platon[2].

Table S17. Selected hypothetical low-energy crystal structures of **DDS Dichloromethane Monosolvate**. Isostructural **SACO** (M2) and **SDCE** (M4) packings differing in solvent molecule orientations are highlighted in colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
3304	*Pbca*	8.347	16.911	21.402	90	90	90	–162.43	12.44	–246.56	0.00	–238.68	0.00	70	
17	$P2_1/n$	5.594	12.120	22.259	90	90.51	90	–174.86	0.00	–237.88	8.68	–230.84	7.85	70.3	M2
37	$P2_1$	5.768	7.680	16.857	90	94.19	90	–171.94	2.92	–237.00	9.56	–229.73	8.95	71.4	
7578	$P2_1$	5.742	7.760	16.856	90	94.20	90	–169.70	5.16	–236.37	10.19	–231.08	7.60	70.9	
481	$P2_1$	5.956	7.804	16.510	90	96.92	90	–171.09	3.77	–235.84	10.72	–232.00	6.68	69.7	
7518	$P2_12_12_1$	10.680	11.550	12.453	90	90	90	–165.00	9.86	–235.19	11.37	–230.61	8.07	68.9	
297	$P2_1/n$	5.699	7.746	34.156	90	94.661	90	–168.74	6.12	–235.13	11.43	–229.66	9.02	70.7	
156	*Pbca*	8.601	16.235	22.649	90	90	90	–167.28	7.58	–235.06	11.50	–229.14	9.55	66.8	M4
4356	$P2_1/c$	8.725	11.445	15.912	90	101.778	90	–166.30	8.56	–233.96	12.60	–225.59	13.09	67.9	
1485	$P2_1/c$	17.650	5.493	15.778	90	96.919	90	–173.54	1.33	–232.86	13.70	–226.23	12.45	69.8	
4210	$P2_1$	5.970	12.659	10.653	90	102.207	90	–165.57	9.29	–232.18	14.38	–225.36	13.32	67.3	
6126	$Pna2_1$	33.737	5.863	7.735	90	90.000	90	–168.39	6.47	–231.81	14.75	–227.36	11.32	69.4	
43	$P2_1/c$	17.660	5.980	15.649	90	112.112	90	–168.69	6.17	–231.45	15.11	–225.05	13.63	69.3	
9479	$P2_1/c$	11.178	7.990	17.323	90	97.985	90	–165.32	9.54	–231.18	15.37	–222.48	16.20	69.3	
2565	$P2_12_12_1$	10.803	11.894	12.154	90	90	90	–165.32	9.54	–231.14	15.41	–228.13	10.55	67.7	
585	$P2_12_12_1$	10.256	11.733	12.677	90	90	90	–165.01	9.85	–230.92	15.63	–228.32	10.36	69.6	
1973	$P2_1$	5.632	7.678	17.601	90	95.14	90	–167.51	7.35	–230.85	15.71	–225.78	12.90	70.2	
121	$Pna2_1$	34.124	5.644	7.789	90	90	90	–168.21	6.66	–230.84	15.71	–224.83	13.85	71	
1988	$Pna2_1$	34.856	5.674	7.698	90	90	90	–167.04	7.82	–230.38	16.18	–225.80	12.88	69.8	
6632	$P2_1/n$	5.631	7.656	35.305	90	93.889	90	–167.69	7.17	–229.85	16.71	–225.12	13.56	70.2	
1031	$P2_1$	6.023	7.928	16.311	90	100.47	90	–166.14	8.72	–229.78	16.77	–226.59	12.09	69.4	
365	*Pbca*	5.638	15.744	34.844	90	90	90	–167.30	7.56	–229.25	17.31	–224.94	13.74	68.7	
568	$P2_12_12_1$	5.784	7.856	33.720	90	90	90	–167.30	7.56	–229.21	17.34	–224.08	14.60	69.2	
1112	$P2_12_12_1$	5.694	7.636	34.871	90	90	90	–167.06	7.80	–229.13	17.43	–223.02	15.66	70.2	
57	$P2_12_12_1$	5.640	7.740	34.439	90	90	90	–167.54	7.32	–228.59	17.97	–223.53	15.15	70.9	
876	$P2_1$	5.747	7.710	17.584	90	99.05	90	–164.57	10.29	–228.13	18.42	–222.57	16.11	69	
513	$Pna2_1$	33.429	5.965	7.744	90	90	90	–165.37	9.49	–226.38	20.18	–222.85	15.83	68.8	
1046	$P2_1$	5.374	13.018	11.469	90	101.314	90	–167.05	7.81	–225.85	20.71	–220.18	18.50	67.1	
2733	*Pbca*	8.552	16.551	23.167	90	90	90	–161.54	13.32	–224.76	21.80	–220.72	17.97	64.5	
2784	*Pbca*	8.528	16.561	23.253	90	90	90	–161.51	13.35	–224.43	22.13	–220.34	18.34	64.4	
103	$P2_1/n$	5.549	12.592	22.229	90	90.002	90	–166.52	8.34	–222.76	23.80	–217.27	21.41	68.3	M2

[a]Rank CrystalPredictor; [b]calculated using Platon[2].

Table S18. Selected hypothetical low-energy crystal structures of **DDS Chloroform Monosolvate**. Isostructural **SACO** (M2) and **SDCE** (M4) packings differing in solvent molecule orientations are highlighted in colour.

Str. ID[a]	Space group	Cell parameters						CryOpt		PBE-TS		PBE-D2		PI (PBE-X)	Solvate Class
		a	b	c	α	β	γ	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}	E_{latt}	ΔE_{latt}		
		/Å			/°			/kJ mol^{-1}						/% [b]	
14	*Ia*	15.710	5.909	18.395	90	99.83	90	–171.07	2.70	–239.03	0.00	–232.33	0.00	67.1	
397	*Pbca*	5.874	12.640	11.440	90	102.43	90	–161.36	12.41	–238.94	0.09	–231.07	1.26	68.9	M4
446	$P2_1$	5.897	8.029	33.845	90	90	90	–173.78	0.00	–238.84	0.19	–230.89	1.43	70.9	
78	$P2_12_12_1$	5.869	7.958	17.300	90	91.84	90	–166.06	7.72	–234.20	4.83	–230.85	1.48	68.9	
184	$P2_1/n$	16.132	5.696	18.259	90	98.68	90	–172.00	1.77	–237.87	1.16	–230.83	1.49	69.7	M2
28	$P2_1$	5.693	22.181	13.133	90	95.23	90	–170.82	2.95	–235.14	3.88	–229.91	2.42	67.5	
69	*Ia*	16.735	5.782	17.887	90	112.90	90	–167.55	6.23	–232.74	6.29	–229.08	3.24	65.7	
162	*Ic*	5.943	7.804	34.788	90	94.73	90	–167.41	6.37	–232.30	6.73	–228.60	3.72	65.4	
3136	$P2_1/c$	5.743	7.774	17.710	90	91.04	90	–166.78	6.99	–234.07	4.95	–227.72	4.61	70.0	
564	*Ic*	5.944	7.837	17.247	90	95.31	90	–165.74	8.04	–233.07	5.95	–226.39	5.93	66.1	
96	P21	16.612	5.734	16.925	90	95.47	90	–169.15	4.63	–233.25	5.77	–226.16	6.17	67.0	
784	P212121	5.871	12.424	11.767	90	102.54	90	–166.74	7.04	–230.63	8.40	–226.11	6.21	69.8	
648	$P2_1$	6.050	7.977	17.015	90	95.94	90	–167.15	6.63	–230.53	8.50	–226.05	6.28	69.3	
423	*Ia*	5.837	8.643	8.941	81.66	88.67	73.12	–168.49	5.29	–230.35	8.68	–225.73	6.60	67.0	
110	*Cc*	5.742	13.136	22.057	90	90.21	90	–168.06	5.71	–230.48	8.54	–225.15	7.17	67.4	
1052	*C*2	24.622	44.734	5.881	90	90	90	–164.65	9.13	–231.07	7.96	–224.16	8.17	70.4	
359	$P2_1/n$	8.425	32.808	5.888	90	103.96	90	–168.27	5.51	–230.38	8.64	–223.24	9.09	69.6	
348	$P2_1$	5.761	8.575	9.030	82.53	87.97	73.39	–171.43	2.35	–231.13	7.89	–222.83	9.50	70.9	
2488	$P2_1$	17.512	5.764	16.858	90	101.00	90	–167.80	5.98	–230.05	8.97	–222.67	9.65	70.0	
1128	*C*2	5.816	22.318	12.609	90	96.84	90	–164.06	9.72	–227.15	11.87	–222.10	10.22	69.9	
42	$P2_1$	5.747	8.636	9.072	97.19	92.27	109.27	–167.21	6.57	–227.94	11.09	–221.65	10.67	66.4	
282	$P2_1$	15.710	5.909	18.395	90	99.83	90	–165.77	8.00	–225.61	13.42	–221.35	10.98	68.5	
144	*P*1	5.874	12.640	11.440	90	102.43	90	–169.66	4.12	–226.77	12.26	–221.06	11.27	65.2	
220	$P2_1/n$	5.897	8.029	33.845	90	90	90	–164.26	9.52	–224.88	14.14	–220.94	11.39	67.1	
1370	*Fdd*2	5.869	7.958	17.300	90	91.84	90	–165.57	8.21	–228.56	10.47	–220.11	12.21	69.0	
633	$P2_1/c$	16.132	5.696	18.259	90	98.68	90	–164.67	9.10	–227.13	11.89	–219.27	13.06	71.2	
385	*P*1	5.693	22.181	13.133	90	95.23	90	–167.21	6.57	–222.94	16.08	–219.12	13.21	68.5	
244	$P2_1/c$	16.735	5.782	17.887	90	112.90	90	–164.49	9.29	–222.06	16.96	–217.77	14.55	67.0	
161	$P2_1/n$	5.943	7.804	34.788	90	94.73	90	–164.42	9.36	–223.97	15.06	–216.11	16.21	69.0	
5233	*P*1	5.743	7.774	17.710	90	91.04	90	–164.45	9.33	–220.26	18.76	–215.72	16.61	66.4	

[a]Rank CrystalPredictor; [b]calculated using Platon[2].

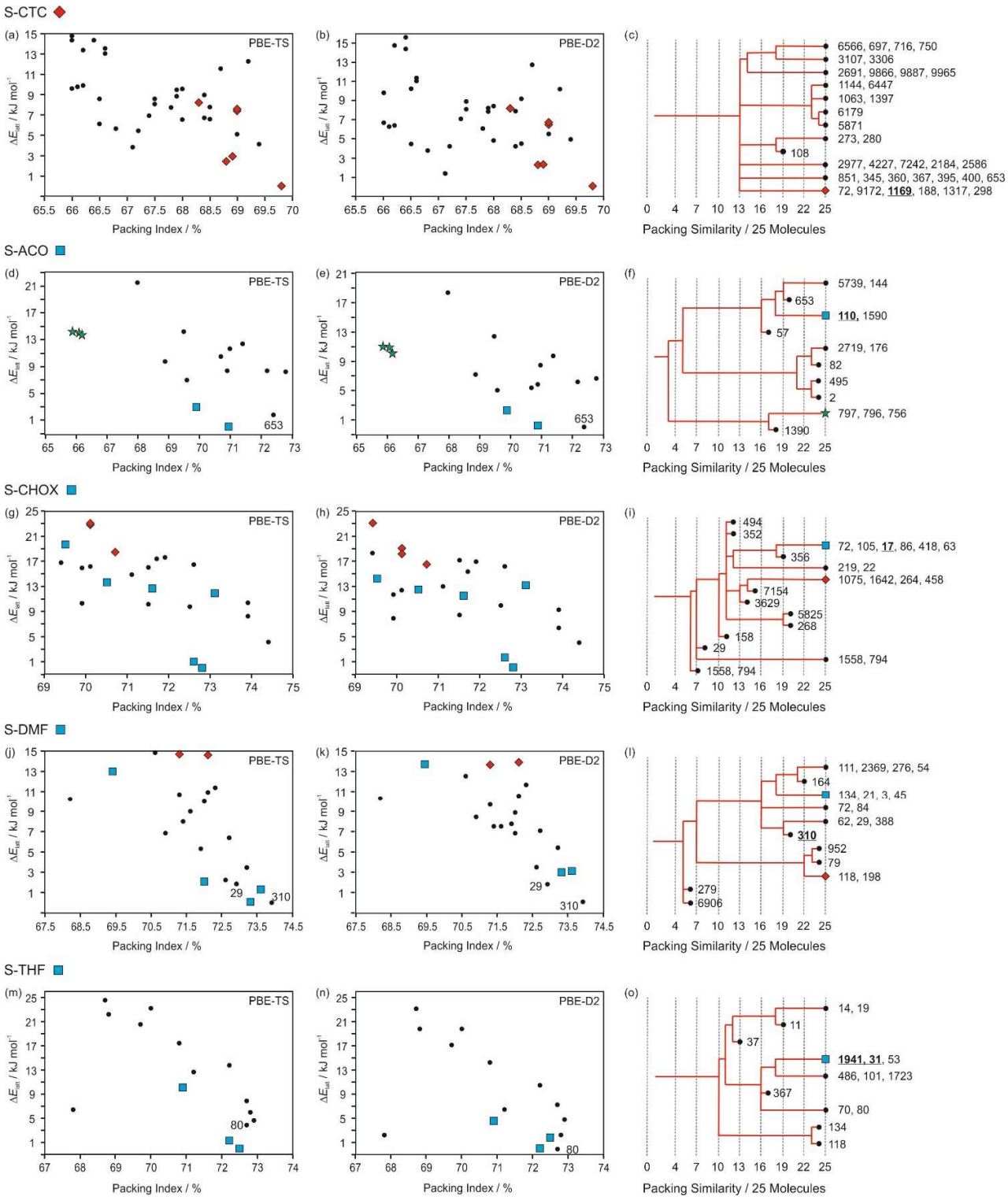


Figure S19. Computationally generated PBE-TS (column 1) and PBE-D2 (column 2) crystal energy landscapes for DDS mono-solvates. Solvate structure family trees (column 3), showing crystal packing similarity between the lowest energy crystal structures from the CSP searches.

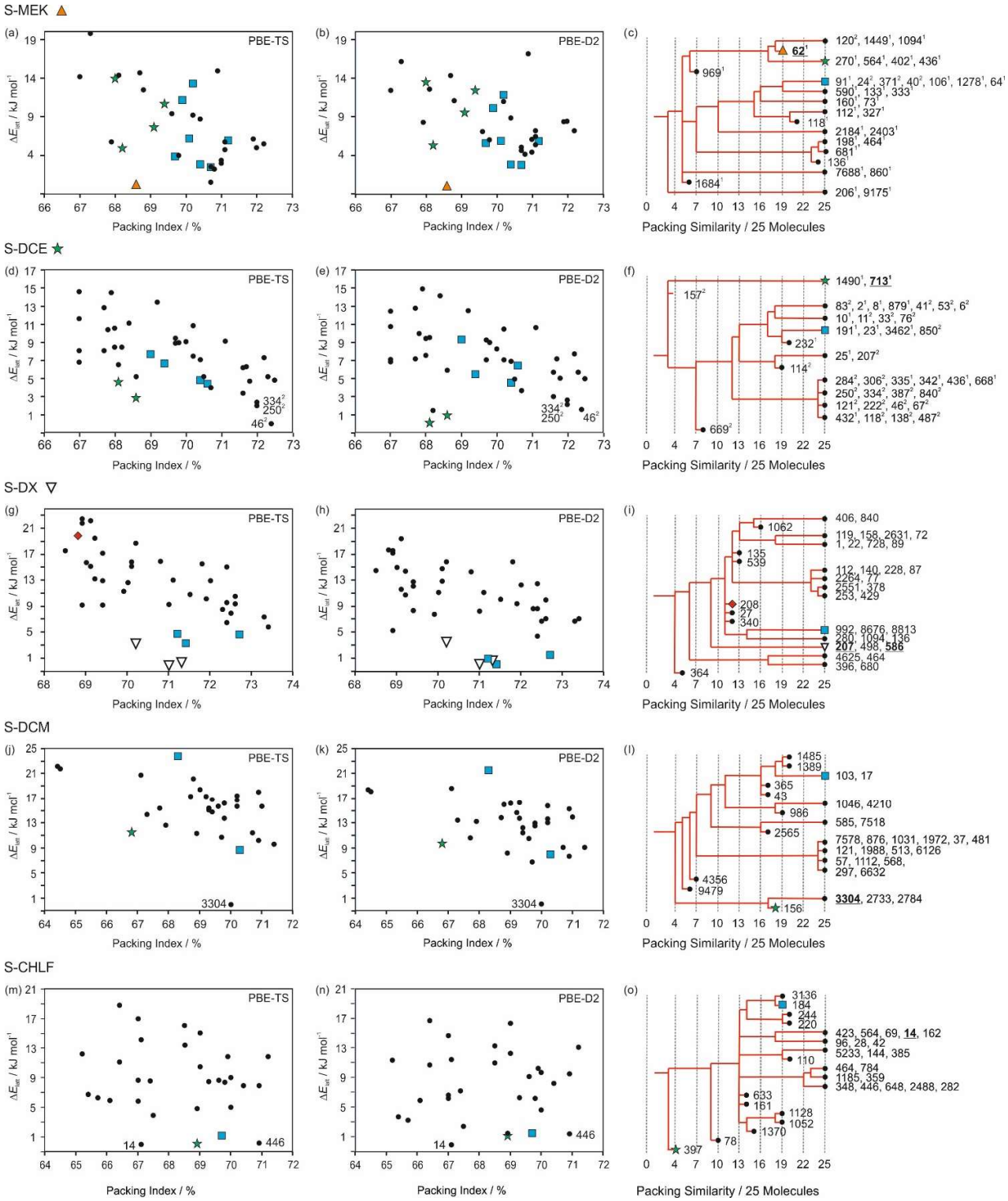


Figure S20. Computationally generated PBE-TS (column 1) and PBE-D2 (column 2) crystal energy landscapes for DDS mono-solvates. Solvate structure family trees (column 3), showing crystal packing similarity between the lowest energy crystal structures from the CSP searches.

4.3. Representation of the Observed Solvate Structures

The computational model was successful in reproducing the experimental solvate structures of **S$_{THF}$** (HASSEB[3]), **S$_{DX}$** (HASSAX[3]) and the DCM hemisolvate (**S$_{0.5DCM}$**, HASRUQ[3]).

The computationally generated low energy structures were compared using the Solid Form module of Mercury to determine the root mean square deviation of the non-hydrogen atoms in a cluster of 15 DDS molecules ($rmsd_{15}$).[4]

Table S19. Quality of Representation of the Experimental DDS Solvate Structures.

Structure	Lattice parameters (cell vectors/Å, angles/°)				Cell Volume (Å^3)	$Rmsd_{15}$ (Å)
	A	*b*	*c*	*β*		
Exptl., **S$_{THF}$**, HASSEB, *P*2$_1$/*n*, 173 K	5.829	12.679	21.808	91.34	1619.46	–
Calc. (PBE-TS), #31, 0 K	5.868	12.232	21.870	92.38	1568.44	0.203
Calc. (PBE-TS), #1941, 0 K	5.623	12.899	21.728	90.78	1575.76	0.224
Exptl., **S$_{DX}$**, HASSAX, *P*bca, 173 K	11.101	11.339	26.628	90	3351.60	–
Calc. (PBE-TS), #207, 0 K	10.895	11.252	26.829	90	3288.91	0.114
Calc. (PBE-TS), #498, 0 K	10.973	11.287	26.911	90	3332.88	0.138
Exptl., **S$_{DCM}$** HASRUQ, *P*2$_1$/*n*, 173 K	8.300	16.599	19.914	98.66	2712.3	–
Calc. (PBE-TS), 0 K	8.276	16.559	19.876	98.92	2691.05	0.038

4.4. Hypothetical Lowest-Energy Monosolvate Structures

4.4.1. Acetone Solvate - #653

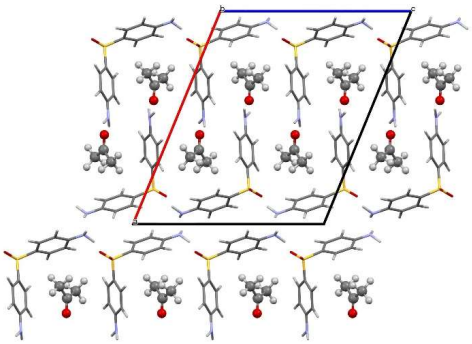


Figure S21. Packing diagram of the Acetone Solvate #653 viewed along the *b* crystallographic axis. Acetone molecules are H-bonded to the amino function of the DDS molecules and arranged in channels in direction of the *b* axis.

4.4.2. DMF Solvate - #310

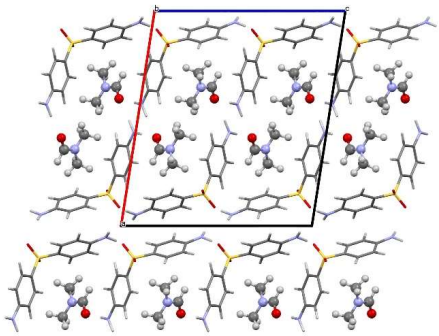


Figure S22. Packing diagram of the DMF Solvate #310 viewed along the *b* crystallographic axis. DMF molecules are H-bonded to the amino function of the DDS molecules and arranged in channels in direction of the *b* axis.

4.4.3. DMF Solvate - #29

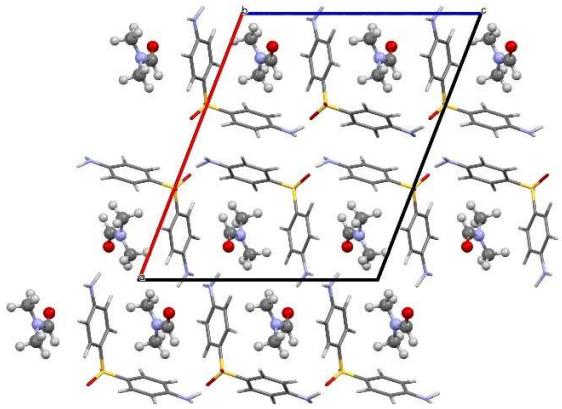


Figure S23. Packing diagram of the DMF Solvate #29 viewed along the *b* crystallographic axis. DMF molecules are H-bonded to the amino function of the DDS molecules and arranged in channels in direction of the *b* axis.

4.4.4. THF Solvate - #80

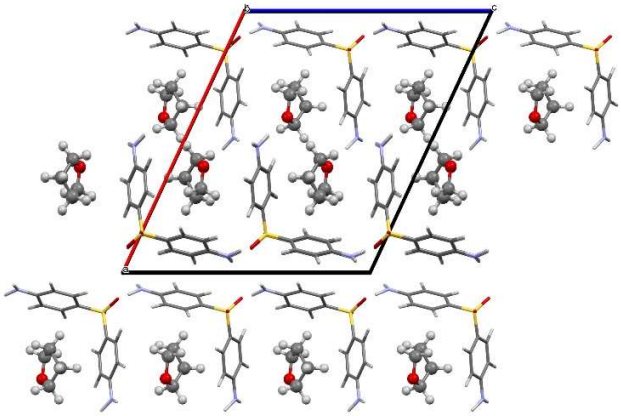


Figure S24. Packing diagram of the THF Solvate #80 viewed along the *b* crystallographic axis. THF molecules are H-bonded to the amino function of the DDS molecules and arranged in channels in direction of the *b* axis. DMF #29 and THF #80 are isostructural.

4.4.5. DCE Solvate - #46[2]

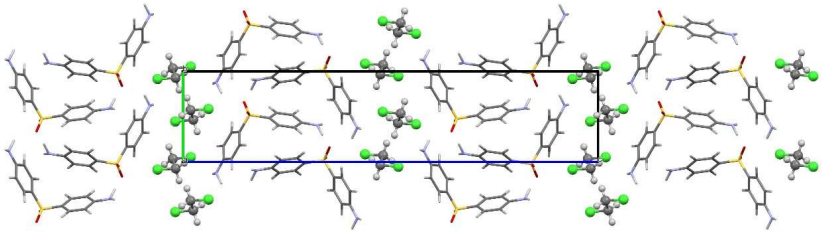


Figure S25. Packing diagram of the DCE Solvate #46[2] viewed along the *a* crystallographic axis. DCE molecules are arranged in layers parallel to (010).

4.4.6. DCE Solvate - #250[2]

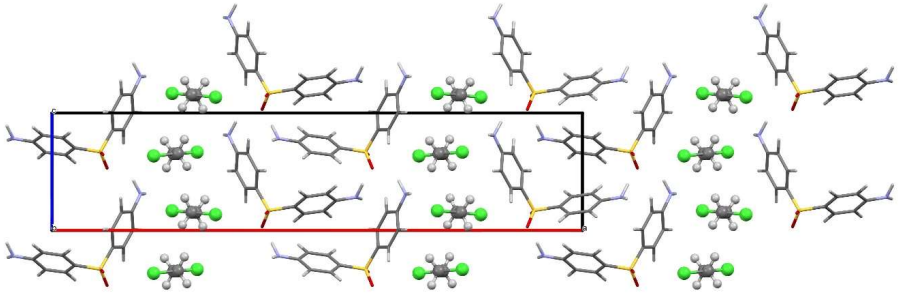


Figure S26. Packing diagram of the DCE Solvate #250[2] viewed along the *b* crystallographic axis. DCE molecules are arranged in layers parallel to (001).

4.4.7. DCE Solvate - #334[2]

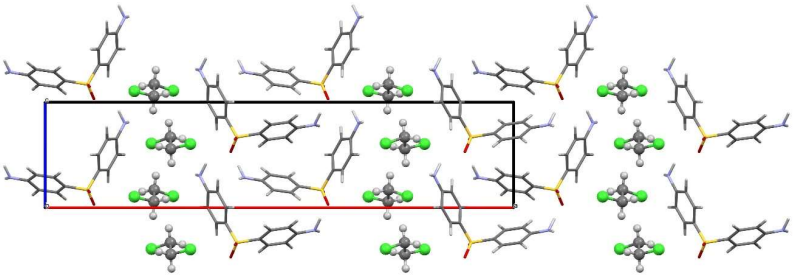


Figure S27. Packing diagram of the DCE Solvate #334[2] viewed along the *b* crystallographic axis. DCE molecules are arranged in layers parallel to (001). DCE #250[2] and #334[2] is isostructural.

4.4.8. Dioxane Solvate - #8676

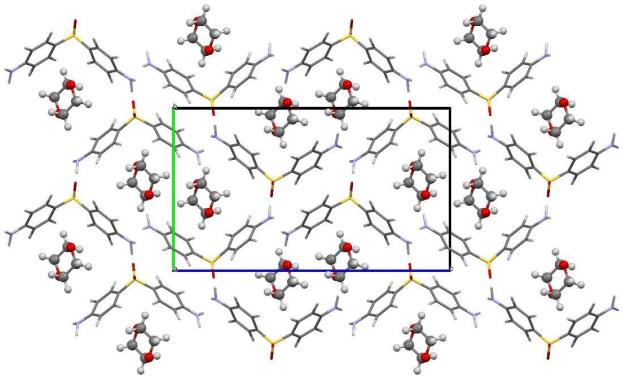


Figure S28. Packing diagram of the Dioxane Solvate #8676 viewed along the *a* crystallographic axis. DMF molecules are H-bonded to the amino function of the DDS molecules and arranged in channels in direction of the *a* axis. DX #8676 belongs to the *M2* structure family.

4.4.9. DCM Solvate - #3304

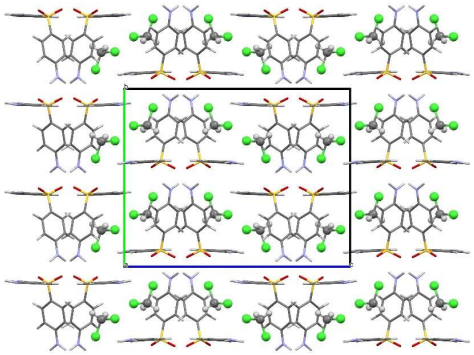


Figure S29. Packing diagram of the DCM Solvate #3304 viewed along the *a* crystallographic axis. DCM molecules are arranged in zig-zag channels in direction of the *a* axis. DCM #3304 and *M4*/*M5* structures show 2D packing similarity.

4.4.10. Chloroform Solvate - #397

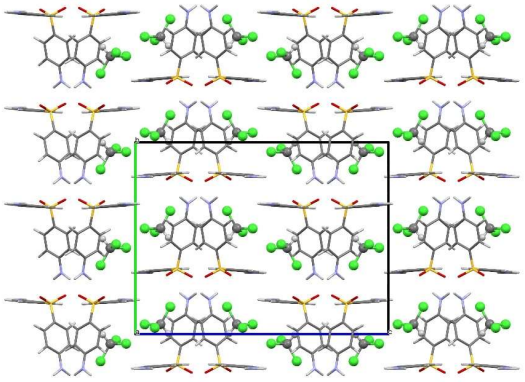


Figure S30. Packing diagram of the CHLF Solvate #397 viewed along the *a* crystallographic axis. CHLF molecules are arranged in zig-zag channels in direction of the *a* axis. CHLF #3304 (M4) and DCM #3304 structures show 2D packing similarity.

4.4.11. Chloroform Solvate - #14

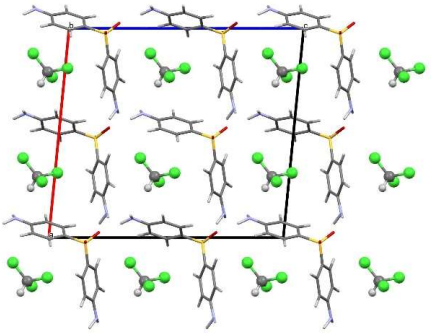


Figure S31. Packing diagram of the CHLF Solvate #14 viewed along the *b* crystallographic axis. CHLF molecules are arranged in channels in direction of the *b* axis.

4.4.12. Chloroform Solvate - #446

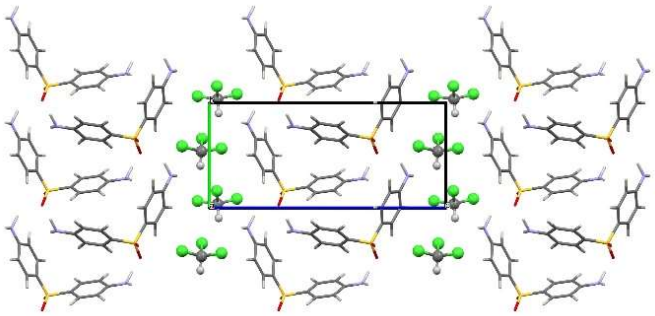


Figure S32. Packing diagram of the CHLF Solvate #446 viewed along the *a* crystallographic axis. CHLF molecules are arranged in channels parallel to the *a* axis. Structures CHLF #446 and DCE #250[2]/#334[2] show 2D similarity.

4.4.13. Chloroform Solvate - #184

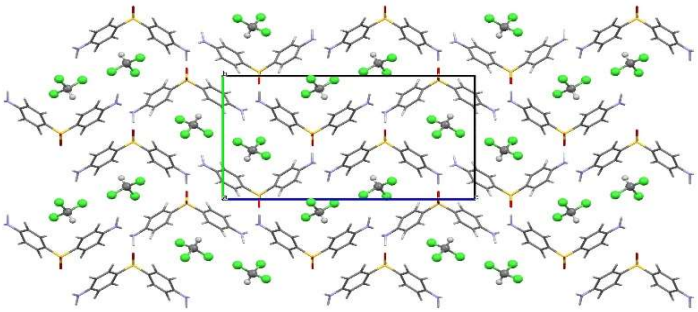


Figure S33. Packing diagram of the CHLF Solvate #184 viewed along the *a* crystallographic axis. CHLF molecules are arranged in channels parallel to the *a* axis. Structure belongs to the *M2* family.

4.5. Computed RT – Structures (.res files)

The .res files of the computationally generated "RT" (lattice parameters fixed during structure optimisation) structures are given below.

4.5.1. SCTC #1169 (PBE-TS)

```
TITL CCl4_RT_1169_TS
CELL  1.54180   5.7875   17.4109    8.7408    90.000   104.812    90.000
ZERR       2    0.0000    0.0000    0.0000     0.000     0.000     0.000
LATT  -1
SYMM           - X ,    0.50000 + Y ,           - Z
SFAC  C  H N  O  S Cl
UNIT    26   24   8   4   4   2
C1    1  0.52935  0.56446  1.19860  11.00000   0.0500
C2    1  0.74846  0.60418  1.22853  11.00000   0.0500
C3    1  0.40086  0.54988  1.04476  11.00000   0.0500
C4    1  0.83336  0.62934  1.10001  11.00000   0.0500
C5    1  0.70598  0.61417  0.94618  11.00000   0.0500
C6    1  0.48883  0.57487  0.91824  11.00000   0.0500
C7    1  0.39514  0.46012  0.68236  11.00000   0.0500
C8    1  0.26260  0.40017  0.72432  11.00000   0.0500
C9    1  0.30776  0.32517  0.68960  11.00000   0.0500
C10   1  0.48521  0.30816  0.60986  11.00000   0.0500
C11   1  0.62075  0.36920  0.57177  11.00000   0.0500
C12   1  0.57773  0.44407  0.60889  11.00000   0.0500
C13   1  0.03922  0.33508  0.17391  11.00000   0.0500
H1    2  0.84951  0.58933  1.47385 11.00000 -1.20000
H2    2  1.04980  0.63724  1.39767 11.00000 -1.20000
H3    2  0.39662  0.19460  0.57841 11.00000 -1.20000
H4    2  0.60539  0.22369  0.48375 11.00000 -1.20000
H5    2  0.46060  0.54538  1.29730 11.00000 -1.20000
H6    2  0.23062  0.51978  1.02260 11.00000 -1.20000
H7    2  1.00247  0.66039  1.12227 11.00000 -1.20000
H8    2  0.77534  0.63216  0.84744 11.00000 -1.20000
H9    2  0.12138  0.41270  0.78217 11.00000 -1.20000
H10   2  0.20340  0.27871  0.72185 11.00000 -1.20000
H11   2  0.76066  0.35707  0.51239 11.00000 -1.20000
H12   2  0.68707  0.49042  0.58232 11.00000 -1.20000
N1    3  0.87457  0.62169  1.38153  11.00000   0.0500
N2    3  0.52802  0.23372  0.57462  11.00000   0.0500
O1    4  0.07427  0.55791  0.71648  11.00000   0.0500
O2    4  0.41796  0.60536  0.61716  11.00000   0.0500
S1    5  0.32888  0.55489  0.72291  11.00000   0.0500
Cl1   6 -0.16383  0.34019 -0.01576  11.00000   0.0500
Cl2   6 -0.02961  0.25272  0.27376  11.00000   0.0500
Cl3   6  0.33319  0.32744  0.15215  11.00000   0.0500
Cl4   6  0.01312  0.41908  0.28292  11.00000   0.0500
END
```

4.5.2. SACO #110 (PBE-TS)

```
TITL ACO_110_RT_TS
CELL  1.54180   5.9775   12.4298   21.7725    90.000    91.377    90.000
ZERR       4    0.0000    0.0000    0.0000     0.000     0.000     0.000
LATT   1
SYMM     0.50000 - X ,    0.50000 + Y ,    0.50000 - Z
SFAC  C  H  N  O  S
C1    1 -0.23207  0.33025  0.22833  11.00000   0.0500
C2    1 -0.18376  0.26678  0.27916  11.00000   0.0500
C3    1  0.02753  0.27290  0.30912  11.00000   0.0500
C4    1  0.18581  0.34623  0.28686  11.00000   0.0500
C5    1  0.13737  0.40964  0.23591  11.00000   0.0500
C6    1 -0.07249  0.40204  0.20636  11.00000   0.0500
C7    1 -0.03983  0.39339  0.07880  11.00000   0.0500
C8    1  0.16483  0.41438  0.05130  11.00000   0.0500
C9    1  0.24163  0.34708  0.00593  11.00000   0.0500
C10   1  0.11812  0.25534 -0.01279  11.00000   0.0500
C11   1 -0.08770  0.23506  0.01582  11.00000   0.0500
C12   1 -0.16543  0.30304  0.06075  11.00000   0.0500
C13   1  0.22102  0.15080  0.16144  11.00000   0.0500
C14   1  0.20571  0.05812  0.11746  11.00000   0.0500
C15   1  0.41063  0.03173  0.08195  11.00000   0.0500
H1    2 -0.00974  0.13868  0.36287 11.00000 -1.20000
H2    2  0.24120  0.20079  0.37168 11.00000 -1.20000
H3    2  0.33454  0.21099 -0.08068 11.00000 -1.20000
H4    2  0.10502  0.12339 -0.07217 11.00000 -1.20000
H5    2 -0.39487  0.32435  0.20517 11.00000 -1.20000
H6    2 -0.30912  0.21128  0.29617 11.00000 -1.20000
H7    2  0.34896  0.35280  0.30991 11.00000 -1.20000
H8    2  0.26318  0.46457  0.21860 11.00000 -1.20000
H9    2  0.26384  0.48359  0.06579 11.00000 -1.20000
H10   2  0.39969  0.36482 -0.01580 11.00000 -1.20000
H11   2 -0.18460  0.16434  0.00226 11.00000 -1.20000
H12   2 -0.32519  0.28649  0.08187 11.00000 -1.20000
H13   2  0.05993  0.16510  0.18265 11.00000 -1.50000
H14   2  0.34873  0.13377  0.19738 11.00000 -1.50000
H15   2  0.27461  0.22412  0.13765 11.00000 -1.50000
H16   2  0.39202 -0.04569  0.05854 11.00000 -1.50000
H17   2  0.43359  0.09472  0.04710 11.00000 -1.50000
H18   2  0.56234  0.03130  0.11145 11.00000 -1.50000
N1    3  0.07472  0.21082  0.36060  11.00000   0.0500
N2    3  0.19810  0.18754 -0.05627  11.00000   0.0500
O1    4  0.00269  0.57356  0.13989  11.00000   0.0500
O2    4 -0.37486  0.48620  0.13322  11.00000   0.0500
O3    4  0.03030  0.00589  0.11074  11.00000   0.0500
S1    5 -0.13124  0.47555  0.13862  11.00000   0.0500
END
```

4.5.3. SCHOX #86 (PBE-TS)

```
TITL CHOX_86_RT_TS
CELL  1.54180   6.0749   13.7461   21.6755    90.000    90.703    90.000
ZERR       4   0.0000    0.0000    0.0000     0.000     0.000     0.000
LATT   1
SYMM     0.50000 - X ,    0.50000 + Y ,    0.50000 - Z
C1    1 -0.22354  0.16858  0.22273  11.00000   0.0500
C2    1 -0.18052  0.23754  0.26790  11.00000   0.0500
C3    1  0.02759  0.24203  0.29728  11.00000   0.0500
C4    1  0.19033  0.17482  0.27954  11.00000   0.0500
C5    1  0.14834  0.10721  0.23351  11.00000   0.0500
C6    1 -0.05960  0.10305  0.20524  11.00000   0.0500
C7    1 -0.02519  0.08287  0.07816  11.00000   0.0500
C8    1  0.18315  0.06687  0.05320  11.00000   0.0500
C9    1  0.25402  0.12290  0.00431  11.00000   0.0500
C10   1  0.12224  0.19881 -0.02022  11.00000   0.0500
C11   1 -0.08974  0.21240  0.00492  11.00000   0.0500
C12   1 -0.16142  0.15545  0.05324  11.00000   0.0500
C13   1  0.09508  0.47992  0.11220  11.00000   0.0500
C14   1  0.11543  0.41481  0.16781  11.00000   0.0500
C15   1  0.35654  0.38462  0.17942  11.00000   0.0500
C16   1  0.45699  0.33969  0.12187  11.00000   0.0500
C17   1  0.44280  0.40909  0.06694  11.00000   0.0500
C18   1  0.20562  0.44399  0.05475  11.00000   0.0500
H1    2 -0.02554  0.37111  0.34383 11.00000 -1.20000
H2    2  0.23088  0.32431  0.35322 11.00000 -1.20000
H3    2  0.34249  0.24146 -0.08754 11.00000 -1.20000
H4    2  0.11003  0.31696 -0.08092 11.00000 -1.20000
H5    2 -0.38510  0.16531  0.20056 11.00000 -1.20000
H6    2 -0.30800  0.28906  0.28120 11.00000 -1.20000
H7    2  0.35065  0.17547  0.30266 11.00000 -1.20000
H8    2  0.27667  0.05686  0.21927 11.00000 -1.20000
H9    2  0.29018  0.01088  0.07258 11.00000 -1.20000
H10   2  0.41515  0.10927 -0.01548 11.00000 -1.20000
H11   2 -0.19824  0.26781 -0.01480 11.00000 -1.20000
H12   2 -0.32535  0.16647  0.07172 11.00000 -1.20000
H13   2  0.01757  0.34855  0.15845 11.00000 -1.20000
H14   2  0.04252  0.45109  0.20775 11.00000 -1.20000
H15   2  0.36285  0.33370  0.21840 11.00000 -1.20000
H16   2  0.45300  0.44882  0.19363 11.00000 -1.20000
H17   2  0.63013  0.32092  0.13119 11.00000 -1.20000
H18   2  0.37141  0.27108  0.11040 11.00000 -1.20000
H19   2  0.54908  0.47273  0.07579 11.00000 -1.20000
H20   2  0.50355  0.37400  0.02483 11.00000 -1.20000
H21   2  0.10747  0.38156  0.03795 11.00000 -1.20000
H22   2  0.19783  0.50048  0.01914 11.00000 -1.20000
N1    3  0.06862  0.30868  0.34379  11.00000   0.0500
N2    3  0.19782  0.25758 -0.06574  11.00000   0.0500
O1    4  0.03390 -0.06387  0.15350  11.00000   0.0500
O2    4 -0.34651  0.00418  0.14075  11.00000   0.0500
O3    4 -0.00609  0.55811  0.11375  11.00000   0.0500
S1    5 -0.10854  0.02028  0.14441  11.00000   0.0500
END
```

4.5.4. SCHOX #105 (PBE-TS)

```
TITL CHOX_105_RT_TS
CELL  1.54180   6.0749   13.7461   21.6755    90.000    90.703    90.000
ZERR       4    0.0000    0.0000    0.0000     0.000     0.000     0.000
LATT   1
SYMM     0.50000 - X ,    0.50000 + Y ,    0.50000 - Z
SFAC  C  H  N  O  S
C1    1  0.67822  0.35159  0.44371  11.00000   0.0500
C2    1  0.60622  0.30534  0.49628  11.00000   0.0500
C3    1  0.39348  0.32382  0.51954  11.00000   0.0500
C4    1  0.26345  0.39538  0.48963  11.00000   0.0500
C5    1  0.33473  0.44053  0.43661  11.00000   0.0500
C6    1  0.54216  0.41842  0.41288  11.00000   0.0500
C7    1  0.56237  0.37837  0.28624  11.00000   0.0500
C8    1  0.34917  0.37287  0.26131  11.00000   0.0500
C9    1  0.29896  0.30196  0.21801  11.00000   0.0500
C10   1  0.45942  0.23478  0.19886  11.00000   0.0500
C11   1  0.67190  0.23987  0.22559  11.00000   0.0500
C12   1  0.72204  0.31084  0.26879  11.00000   0.0500
C13   1  0.11048  0.47699  0.12027  11.00000   0.0500
C14   1  0.06052  0.56180  0.16153  11.00000   0.0500
C15   1  0.12550  0.65736  0.12958  11.00000   0.0500
C16   1  0.36510  0.65574  0.10934  11.00000   0.0500
C17   1  0.41081  0.56964  0.06678  11.00000   0.0500
C18   1  0.34174  0.47229  0.09618  11.00000   0.0500
H1    2  0.39186  0.21082  0.58314 11.00000 -1.20000
H2    2  0.16156  0.28765  0.58492 11.00000 -1.20000
H3    2  0.24789  0.15193  0.14673 11.00000 -1.20000
H4    2  0.50476  0.10458  0.15459 11.00000 -1.20000
H5    2  0.84096  0.33578  0.42582 11.00000 -1.20000
H6    2  0.71280  0.25333  0.52013 11.00000 -1.20000
H7    2  0.10267  0.41335  0.50828 11.00000 -1.20000
H8    2  0.22804  0.49226  0.41294 11.00000 -1.20000
H9    2  0.22318  0.42384  0.27621 11.00000 -1.20000
H10   2  0.13405  0.29822  0.19790 11.00000 -1.20000
H11   2  0.79642  0.18728  0.21186 11.00000 -1.20000
H12   2  0.88595  0.31449  0.28945 11.00000 -1.20000
H13   2  0.15859  0.55415  0.20446 11.00000 -1.20000
H14   2 -0.11406  0.56024  0.17387 11.00000 -1.20000
H15   2  0.09518  0.71860  0.16066 11.00000 -1.20000
H16   2  0.01784  0.66868  0.08902 11.00000 -1.20000
H17   2  0.40313  0.72417  0.08551 11.00000 -1.20000
H18   2  0.47463  0.65226  0.15029 11.00000 -1.20000
H19   2  0.31980  0.57988  0.02294 11.00000 -1.20000
H20   2  0.58656  0.56589  0.05541 11.00000 -1.20000
H21   2  0.45306  0.45685  0.13559 11.00000 -1.20000
H22   2  0.35538  0.41125  0.06385 11.00000 -1.20000
N1    3  0.31680  0.27414  0.56902  11.00000   0.0500
N2    3  0.41188  0.16738  0.15339  11.00000   0.0500
O1    4  0.49368  0.55276  0.32848  11.00000   0.0500
O2    4  0.86576  0.47660  0.34399  11.00000   0.0500
O3    4 -0.03317  0.41701  0.10552  11.00000   0.0500
S1    5  0.62575  0.46675  0.34231  11.00000   0.0500
END
```

4.5.5. S_{DMF} #3 (PBE-TS)

```
TITL DMF_3_RT_TS
CELL  1.54180   6.1019   12.6882   21.3219    90.000    92.211    90.000
ZERR       4   0.0000    0.0000    0.0000     0.000     0.000     0.000
LATT   1
SYMM     0.50000 - X ,    0.50000 + Y ,    0.50000 - Z
SFAC  C  H  N  O  S
UNIT    60   76  12  12   4
C1    1  0.33346  0.17911  0.06138  11.00000   0.0500
C2    1  0.41021  0.24351  0.01478  11.00000   0.0500
C3    1  0.61521  0.22359 -0.01192  11.00000   0.0500
C4    1  0.73613  0.13474  0.00976  11.00000   0.0500
C5    1  0.66002  0.07116  0.05672  11.00000   0.0500
C6    1  0.45799  0.09257  0.08292  11.00000   0.0500
C7    1  0.43255  0.09229  0.21342  11.00000   0.0500
C8    1  0.63965  0.08606  0.24376  11.00000   0.0500
C9    1  0.69135  0.15220  0.29393  11.00000   0.0500
C10   1  0.53869  0.22712  0.31408  11.00000   0.0500
C11   1  0.32932  0.23108  0.28373  11.00000   0.0500
C12   1  0.27762  0.16439  0.23404  11.00000   0.0500
C13   1  0.48714  0.43683  0.13195  11.00000   0.0500
C14   1  0.81489  0.46310  0.07117  11.00000   0.0500
C15   1  0.81768  0.33811  0.16091  11.00000   0.0500
H1    2  0.62971  0.35901 -0.06881 11.00000 -1.20000
H2    2  0.84400  0.26880 -0.07525 11.00000 -1.20000
H3    2  0.75233  0.30497  0.37440 11.00000 -1.20000
H4    2  0.50367  0.36355  0.36400 11.00000 -1.20000
H5    2  0.17504  0.19554  0.08121 11.00000 -1.20000
H6    2  0.31199  0.31054 -0.00160 11.00000 -1.20000
H7    2  0.89224  0.11657 -0.01097 11.00000 -1.20000
H8    2  0.75735  0.00431  0.07333 11.00000 -1.20000
H9    2  0.76020  0.02991  0.22752 11.00000 -1.20000
H10   2  0.85252  0.14751  0.31770 11.00000 -1.20000
H11   2  0.20784  0.28671  0.30007 11.00000 -1.20000
H12   2  0.11545  0.16704  0.21099 11.00000 -1.20000
H13   2  0.42179  0.39097  0.17134 11.00000 -1.20000
H14   2  0.69648  0.50238  0.03920 11.00000 -1.50000
H15   2  0.93769  0.51964  0.08963 11.00000 -1.50000
H16   2  0.90058  0.40218  0.04498 11.00000 -1.50000
H17   2  0.97019  0.37316  0.18042 11.00000 -1.50000
H18   2  0.85715  0.26769  0.13339 11.00000 -1.50000
H19   2  0.71685  0.31393  0.19978 11.00000 -1.50000
N1    3  0.69509  0.28663 -0.05719  11.00000   0.0500
N2    3  0.58842  0.29324  0.36418  11.00000   0.0500
N3    3  0.69885  0.41431  0.12192  11.00000   0.0500
O1    4  0.50196 -0.07945  0.14978  11.00000   0.0500
O3    4  0.13189  0.00629  0.14036  11.00000   0.0500
O3    4  0.37088  0.50103  0.10141  11.00000   0.0500
S1    5  0.37081  0.01646  0.14582  11.00000   0.0500
END
```

4.5.6. S_{DMF} #45 (PBE-TS)

```
TITL DMF_45_RT_TS
CELL  1.54180   6.1019   12.6882   21.3219    90.000    92.211    90.000
ZERR       4   0.0000   0.0000   0.0000     0.000     0.000     0.000
LATT   1
SYMM     0.50000 - X ,    0.50000 + Y ,    0.50000 - Z
SFAC  C  H  N  O  S
UNIT    60   76  12  12   4
C1    1  1.17826  0.32968  0.44172  11.00000   0.0500
C2    1  1.11313  0.25709  0.48543  11.00000   0.0500
C3    1  0.90391  0.26426  0.51157  11.00000   0.0500
C4    1  0.76589  0.34865  0.49216  11.00000   0.0500
C5    1  0.82998  0.42012  0.44747  11.00000   0.0500
C6    1  1.03709  0.41133  0.42197  11.00000   0.0500
C7    1  1.06265  0.41625  0.29239  11.00000   0.0500
C8    1  0.85473  0.41715  0.26233  11.00000   0.0500
C9    1  0.81117  0.35174  0.21137  11.00000   0.0500
C10   1  0.97355  0.28343  0.18938  11.00000   0.0500
C11   1  1.18223  0.28346  0.22024  11.00000   0.0500
C12   1  1.22549  0.34900  0.27109  11.00000   0.0500
C13   1  0.68454  0.00734  0.40819  11.00000   0.0500
C14   1  0.72582  0.16376  0.34303  11.00000   0.0500
C15   1  0.35805  0.08563  0.35746  11.00000   0.0500
H1    2  0.93630  0.12761  0.56499 11.00000 -1.20000
H2    2  0.69512  0.20326  0.57624 11.00000 -1.20000
H3    2  0.77123  0.20587  0.12588 11.00000 -1.20000
H4    2  1.02522  0.15292  0.13504 11.00000 -1.20000
H5    2  1.34083  0.32376  0.42266 11.00000 -1.20000
H6    2  1.22317  0.19345  0.50027 11.00000 -1.20000
H7    2  0.60630  0.35715  0.51276 11.00000 -1.20000
H8    2  0.71914  0.48308  0.43221 11.00000 -1.20000
H9    2  0.72775  0.46942  0.27908 11.00000 -1.20000
H10   2  0.64990  0.35321  0.18756 11.00000 -1.20000
H11   2  1.30961  0.23118  0.20366 11.00000 -1.20000
H12   2  1.38732  0.34894  0.29443 11.00000 -1.20000
H13   2  0.56098 -0.04646  0.42756 11.00000 -1.20000
H14   2  0.89678  0.15296  0.35885 11.00000 -1.50000
H15   2  0.67364  0.24339  0.35608 11.00000 -1.50000
H16   2  0.71096  0.15609  0.29163 11.00000 -1.50000
H17   2  0.28857  0.16381  0.36604 11.00000 -1.50000
H18   2  0.32641  0.06569  0.30767 11.00000 -1.50000
H19   2  0.27275  0.02886  0.38649 11.00000 -1.50000
N1    3  0.83953  0.19220  0.55428  11.00000   0.0500
N2    3  0.93324  0.22092  0.13713  11.00000   0.0500
N3    3  0.59199  0.08526  0.37309  11.00000   0.0500
O1    4  0.97172  0.58475  0.35665  11.00000   0.0500
O2    4  1.35150  0.50937  0.36617  11.00000   0.0500
O4    4  0.88509 -0.00564  0.41865  11.00000   0.0500
S1    5  1.11423  0.49269  0.36036  11.00000   0.0500
END
```

4.5.7. SMEK #62[1] (PBE-TS)

```
TITL MEK_62-1_RT_TS
CELL  1.54180   8.6083   16.3216   25.0261    90.000    90.000    90.000
ZERR       8    0.0000    0.0000    0.0000     0.000     0.000     0.000
LATT   1
SYMM     0.50000 - X ,          - Y ,    0.50000 + Z
SYMM     0.50000 + X ,    0.50000 - Y ,          - Z
SYMM           - X ,    0.50000 + Y ,    0.50000 - Z
SFAC  C  H  N  O  S
C1    1  0.15317  0.56132  0.13633  11.00000   0.0500
C2    1  0.15774  0.56196  0.08036  11.00000   0.0500
C3    1  0.29855  0.56537  0.05395  11.00000   0.0500
C4    1  0.43951  0.56690  0.08295  11.00000   0.0500
C5    1  0.43248  0.56064  0.13921  11.00000   0.0500
C6    1  0.29196  0.55880  0.16564  11.00000   0.0500
C7    1 -0.07507  0.46033  0.18131  11.00000   0.0500
C8    1 -0.18100  0.41992  0.14799  11.00000   0.0500
C9    1 -0.21043  0.33743  0.15530  11.00000   0.0500
C10   1 -0.13373  0.29272  0.19595  11.00000   0.0500
C11   1 -0.02460  0.33440  0.22842  11.00000   0.0500
C12   1  0.00365  0.41673  0.22139  11.00000   0.0500
C13   1  0.30210  0.32752  0.08137  11.00000   0.0500
C14   1  0.11232  0.32011  0.00283  11.00000   0.0500
C15   1  0.13728  0.31501  0.06278  11.00000   0.0500
C16   1  0.33669  0.30246  0.13767  11.00000   0.0500
H1    2  0.04972  0.56151  0.05779 11.00000 -1.20000
H2    2  0.30219  0.56762  0.01044 11.00000 -1.20000
H3    2  0.53998  0.55967  0.16207 11.00000 -1.20000
H4    2  0.29070  0.55722  0.20912 11.00000 -1.20000
H5    2 -0.24057  0.45314  0.11627 11.00000 -1.20000
H6    2 -0.29258  0.30619  0.12917 11.00000 -1.20000
H7    2  0.03813  0.30030  0.25896 11.00000 -1.20000
H8    2  0.08805  0.44764  0.24685 11.00000 -1.20000
H9    2  0.67488  0.58562  0.08048 11.00000 -1.20000
H10   2  0.58344  0.59329  0.01851 11.00000 -1.20000
H11   2 -0.10437  0.17948  0.23246 11.00000 -1.20000
H12   2 -0.23671  0.18064  0.17933 11.00000 -1.20000
H13   2  0.18675  0.27671 -0.01892 11.00000 -1.50000
H14   2  0.13857  0.38177 -0.01216 11.00000 -1.50000
H15   2 -0.00868  0.30575 -0.00725 11.00000 -1.50000
H16   2  0.06752  0.36185  0.08381 11.00000 -1.20000
H17   2  0.09481  0.25648  0.07919 11.00000 -1.20000
H18   2  0.34628  0.23520  0.13909 11.00000 -1.50000
H19   2  0.24183  0.31920  0.16484 11.00000 -1.50000
H20   2  0.44580  0.32967  0.15106 11.00000 -1.50000
N1    3  0.57903  0.57367  0.05759  11.00000   0.0500
N2    3 -0.16398  0.21233  0.20420  11.00000   0.0500
O1    4  0.00010  0.60104  0.22197  11.00000   0.0500
O2    4 -0.14145  0.59905  0.13479  11.00000   0.0500
O3    4  0.40428  0.35640  0.05209  11.00000   0.0500
S1    5 -0.02447  0.56235  0.17004  11.00000   0.0500
END
```

4.5.8. S_{DCE} #713[1] (PBE-TS)

```
TITL DCE_713-1_RT_TS
CELL 0.71073 8.6757 16.7584 23.1275 90 90 90
ZERR 8 0.0000 0.0000 0.0000 0 0 0
LATT 1
SYMM 1/2-x,-y,1/2+z
SYMM 1/2+x,1/2-y,-z
SYMM -x,1/2+y,1/2-z
SFAC C H N O S Cl
C1     1  0.496590  0.052920  0.228410  1.000000 0.05000
C2     1  0.642910 -0.066830  0.205020  1.000000 0.05000
C3     1  0.533890 -0.025850  0.239560  1.000000 0.05000
C4     1  0.711020 -0.025210  0.158510  1.000000 0.05000
C5     1  0.673360  0.053330  0.147250  1.000000 0.05000
C6     1  0.567010  0.093470  0.182310  1.000000 0.05000
C7     1  0.341060  0.192670  0.131250  1.000000 0.05000
C8     1  0.332760  0.185510  0.070940  1.000000 0.05000
C9     1  0.191090  0.183660  0.043570  1.000000 0.05000
C10    1  0.052660  0.188850  0.075730  1.000000 0.05000
C11    1  0.063560  0.195970  0.136490  1.000000 0.05000
C12    1  0.205020  0.197440  0.163730  1.000000 0.05000
C13    1  0.167420  0.412340  0.106300  1.000000 0.05000
C14    1  0.292050  0.474500  0.110280  1.000000 0.05000
H1     2  0.617740 -0.178440  0.243760  1.000000 0.06000
H2     2  0.748380 -0.174540  0.186950  1.000000 0.06000
H3     2 -0.098990  0.170560  0.007530  1.000000 0.06000
H4     2 -0.185720  0.195690  0.073390  1.000000 0.06000
H5     2  0.411930  0.082820  0.255660  1.000000 0.06000
H6     2  0.476320 -0.057550  0.274550  1.000000 0.06000
H7     2  0.793130 -0.055710  0.130590  1.000000 0.06000
H8     2  0.726840  0.083510  0.110750  1.000000 0.06000
H9     2  0.437560  0.182760  0.045140  1.000000 0.06000
H10    2  0.186500  0.180110 -0.003470  1.000000 0.06000
H11    2 -0.041160  0.200710  0.162190  1.000000 0.06000
H12    2  0.208810  0.203500  0.210500  1.000000 0.06000
H13    2  0.075080  0.427880  0.136580  1.000000 0.06000
H14    2  0.209410  0.352310  0.116280  1.000000 0.06000
H15    2  0.330840  0.480340  0.155270  1.000000 0.06000
H16    2  0.252190  0.532700  0.094810  1.000000 0.06000
N1     3  0.681910 -0.144010  0.216030  1.000000 0.05000
N2     3 -0.087430  0.188800  0.049410  1.000000 0.05000
O1     4  0.636560  0.225550  0.128430  1.000000 0.05000
O2     4  0.495490  0.233670  0.222380  1.000000 0.05000
S1     5  0.518510  0.193080  0.167110  1.000000 0.05000
Cl1    6  0.081680  0.408640  0.036190  1.000000 0.05000
Cl2    6  0.457470  0.449530  0.067710  1.000000 0.05000
END
```

4.5.9. S_{DCE} #1490[1] (PBE-TS)

```
TITL DCE_1490-1_RT_TS
CELL 0.71073 8.6757 16.7576 23.1301 90 90 90
ZERR 8 0.0000 0.0000 0.0000 0 0 0
LATT 1
SYMM 1/2-x,-y,1/2+z
SYMM 1/2+x,1/2-y,-z
SYMM -x,1/2+y,1/2-z
SFAC C H N O S Cl
UNIT 112 128 16 16 8 16
C1     1  1.004400  0.043750  0.226270  1.000000 0.05000
C2     1  1.040410 -0.035160  0.236780  1.000000 0.05000
C3     1  1.151010 -0.075730  0.202760  1.000000 0.05000
C4     1  1.226410 -0.032460  0.158590  1.000000 0.05000
C5     1  1.191080  0.046800  0.148430  1.000000 0.05000
C6     1  1.078760  0.085400  0.181660  1.000000 0.05000
C7     1  0.845830  0.179720  0.130030  1.000000 0.05000
C8     1  0.838480  0.167580  0.070160  1.000000 0.05000
C9     1  0.698110  0.170720  0.041890  1.000000 0.05000
C10    1  0.560570  0.186390  0.072680  1.000000 0.05000
C11    1  0.569710  0.195240  0.133320  1.000000 0.05000
C12    1  0.710060  0.192340  0.161440  1.000000 0.05000
C13    1  0.622480  0.426790  0.074570  1.000000 0.05000
C14    1  0.744370  0.441090  0.119810  1.000000 0.05000
H1     2  1.121070 -0.186580  0.241850  1.000000 0.06000
H2     2  1.257620 -0.184440  0.186610  1.000000 0.06000
H3     2  0.411850  0.178150  0.002620  1.000000 0.06000
H4     2  0.323300  0.200490  0.068180  1.000000 0.06000
H5     2  0.918370  0.073430  0.253020  1.000000 0.06000
H6     2  0.982670 -0.067180  0.271520  1.000000 0.06000
H7     2  1.314050 -0.061660  0.132330  1.000000 0.06000
H8     2  1.251070  0.078990  0.114340  1.000000 0.06000
H9     2  0.943470  0.156990  0.045540  1.000000 0.06000
H10    2  0.693430  0.162000 -0.004780  1.000000 0.06000
H11    2  0.465020  0.205450  0.158190  1.000000 0.06000
H12    2  0.713090  0.201320  0.207980  1.000000 0.06000
H13    2  0.520410  0.462880  0.084510  1.000000 0.06000
H14    2  0.589430  0.363680  0.072480  1.000000 0.06000
H15    2  0.699980  0.423110  0.162270  1.000000 0.06000
H16    2  0.780450  0.503710  0.121420  1.000000 0.06000
N1     3  1.185080 -0.153580  0.213280  1.000000 0.05000
N2     3  0.423020  0.195300  0.044790  1.000000 0.05000
O1     4  1.139640  0.217430  0.126860  1.000000 0.05000
O2     4  0.997990  0.225050  0.220780  1.000000 0.05000
S1     5  1.023760  0.183710  0.166000  1.000000 0.05000
Cl1    6  0.685220  0.455170  0.003990  1.000000 0.05000
Cl2    6  0.913080  0.382250  0.107020  1.000000 0.05000
END
```

5. Pair-wise Intermolecular Energy Calculations

The pair-wise energy contributions to DDS solvate structures, CASTEP RT models, are depicted *via* energy frameworks. Cylinders with thickness proportional to the magnitude of the interaction energy link the centres of mass of the molecules. Figure S34 to Figure S41 show the total energies. The energy contributions are also given in Table S20.

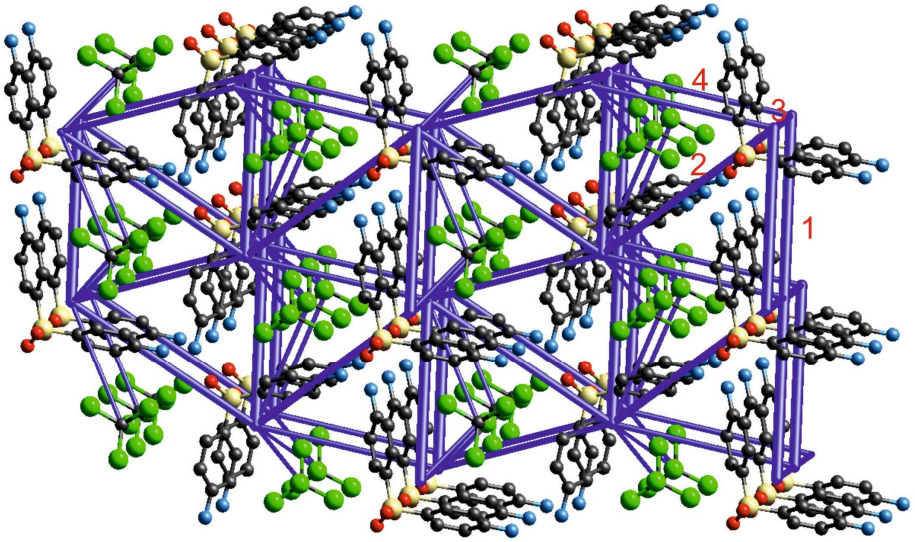


Figure S34. Energy frameworks (total energy) for **S**$_{CTC}$ (#1169). The energy scale factor is 80; interaction energies with magnitudes smaller than 10 kJ mol^{-1} have been omitted. Strongest pair-wise interactions are indicated with red numbers (Table S20).

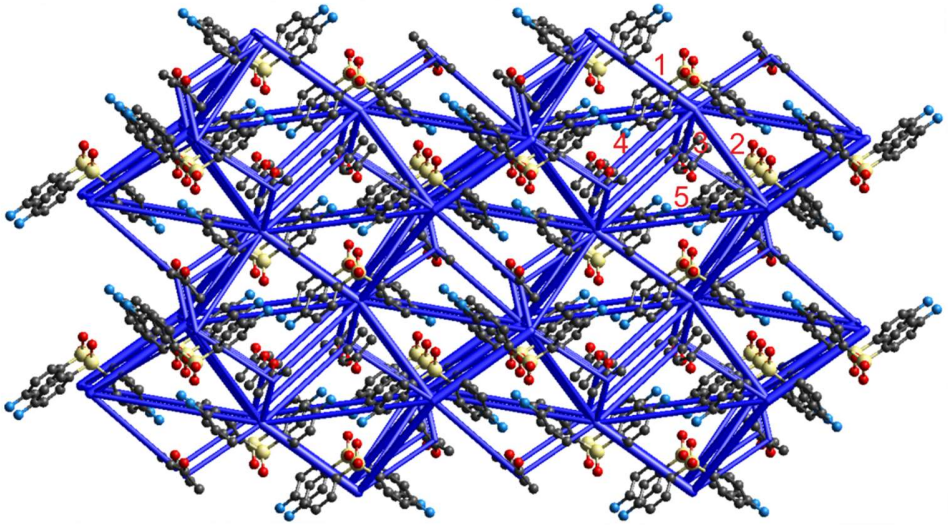


Figure S35. Energy frameworks (total energy) for **S**$_{ACO}$ (#110). The energy scale factor is 80; interaction energies with magnitudes smaller than 10 kJ mol^{-1} have been omitted. Strongest pair-wise interactions are indicated with red numbers (Table S20).

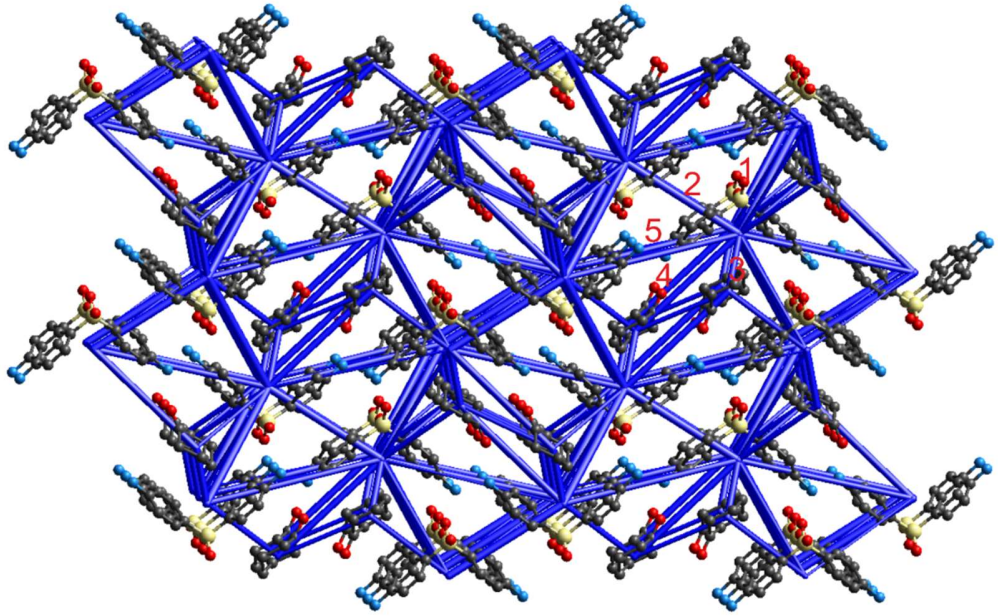


Figure S36. Energy frameworks (total energy) for **SCHOX** (#17). The energy scale factor is 80; interaction energies with magnitudes smaller than 10 kJ mol^{-1} have been omitted. Strongest pair-wise interactions are indicated with red numbers (Table S20).

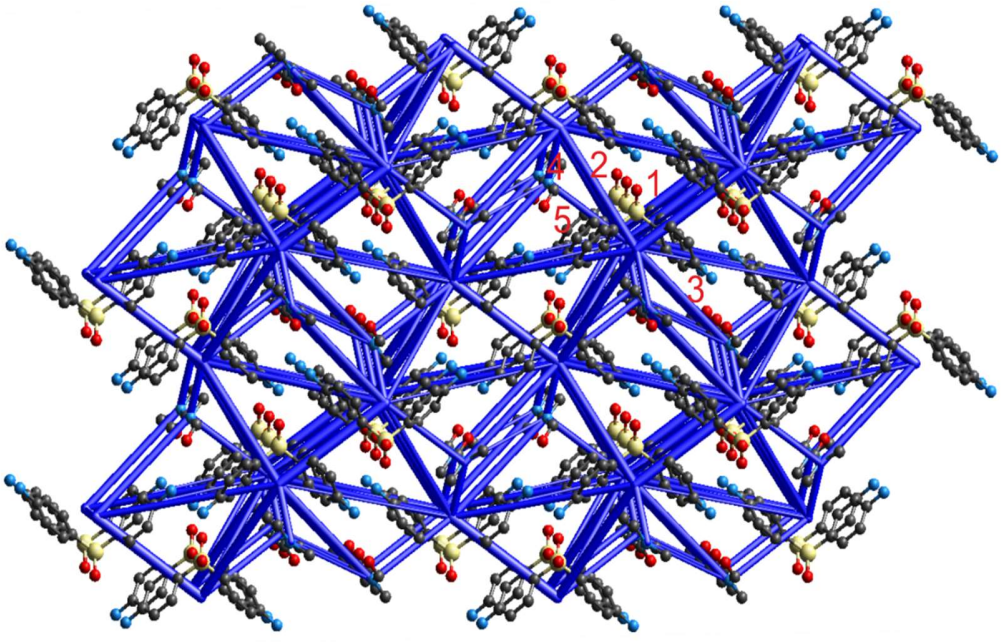


Figure S37. Energy frameworks (total energy) for **SDMF** (#3). The energy scale factor is 80; interaction energies with magnitudes smaller than 10 kJ mol^{-1} have been omitted. Strongest pair-wise interactions are indicated with red numbers (Table S20).

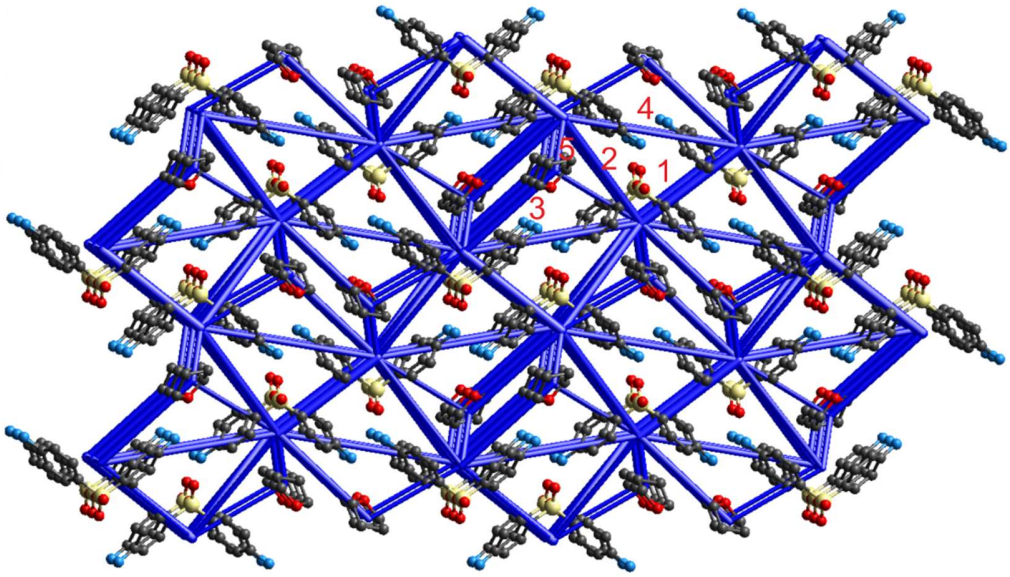


Figure S38. Energy frameworks (total energy) for **STHF** (#1941). The energy scale factor is 80; interaction energies with magnitudes smaller than 10 kJ mol^{-1} have been omitted. Strongest pair-wise interactions are indicated with red numbers (Table S20).

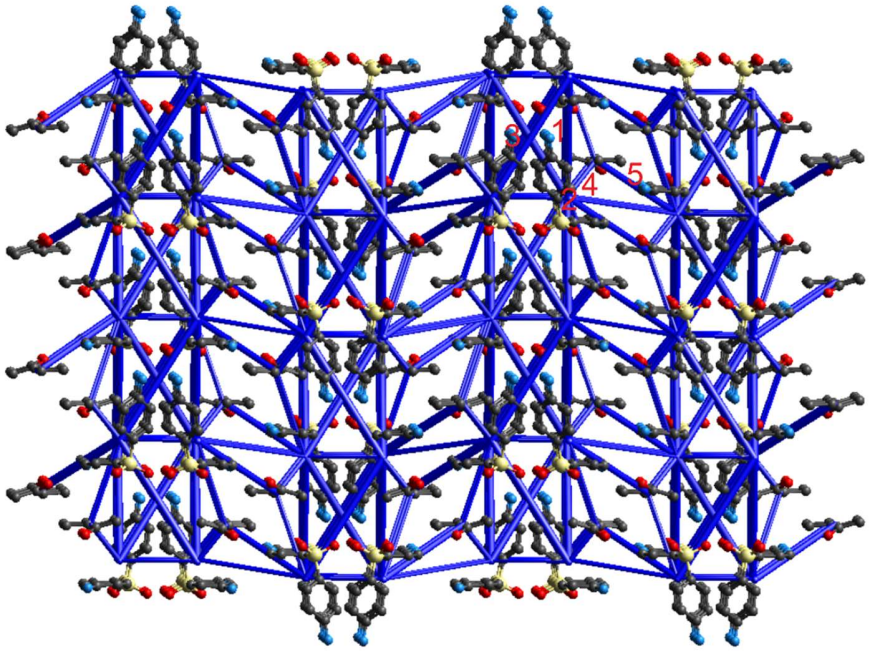


Figure S39. Energy frameworks (total energy) for **SMEK** (#62[1]). The energy scale factor is 80; interaction energies with magnitudes smaller than 10 kJ mol^{-1} have been omitted. Strongest pair-wise interactions are indicated with red numbers (Table S20).

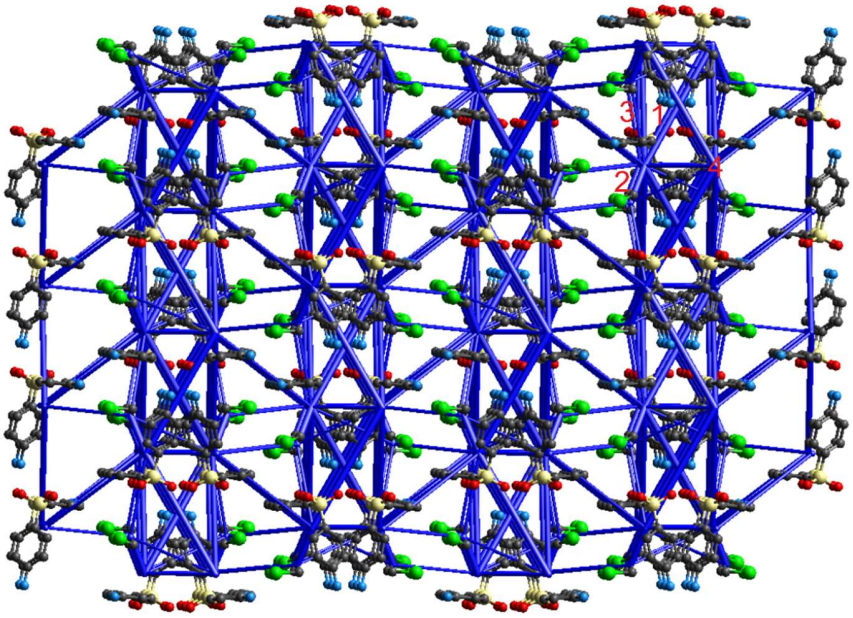


Figure S40. Energy frameworks (total energy) for **S$_{DCE}$** (#713[1]). The energy scale factor is 80; interaction energies with magnitudes smaller than 10 kJ mol^{-1} have been omitted. Strongest pair-wise interactions are indicated with red numbers (Table S20).

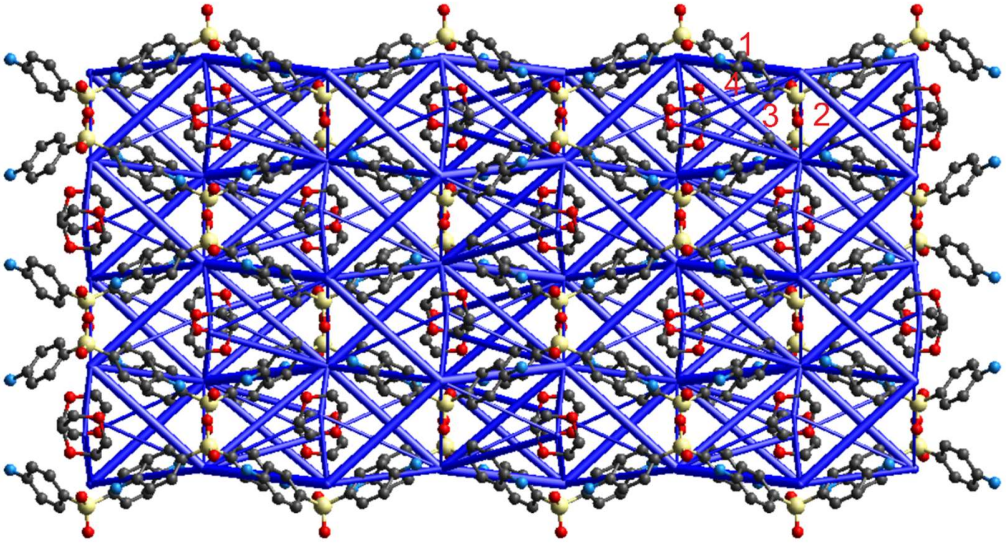


Figure S41. Energy frameworks (total energy) for **S$_{DX}$** (#207). The energy scale factor is 80; interaction energies with magnitudes smaller than 10 kJ mol^{-1} have been omitted. Strongest pair-wise interactions are indicated with red numbers (Table S20).

Table S20. Pair-wise intermolecular interaction energies[a] of **DDS Monosolvates** (ordered PBE-TS RT structures).

Inter-action	Molecules Involved	Distance (Å)	E_E (kJ mol^{-1})	E_P (kJ mol^{-1})	E_D (kJ mol^{-1})	E_R (kJ mol^{-1})	E_{tot}[b] (kJ mol^{-1})
S-CTC (#1169_RT), $E_{cluster}$ = –173.5 kJ mol^{-1}							
1 (2)	DDS···DDS	9.17	–30	–6.2	–11.3	17.1	–35.6
2 (2)	DDS···DDS	10.49	–22.1	–5.2	–6.9	13.4	–24.9
3 (2)	DDS···DDS	5.79	–1.4	–6.1	–27	16.9	–19.1
4 (2)	DDS···DDS	9.17	–17.8	–4.9	–17.7	31	–18.8
5 (2)	DDS···CTC	6.37	–4.1	–1.4	–21.2	15.1	–14.5
6 (2)	DDS···CTC	4.73	–3.8	–0.8	–21.8	16.7	–13.3
7 (2)	DDS···CTC	5.28	–2.7	–0.2	–15.6	8.7	–11.2
8 (2)	DDS···CTC	6.58	–2.8	–1.4	–8.1	4.5	–8.3
9 (2)	DDS···CTC	6.44	–1.7	–0.7	–11.4	7.6	–7.6
10 (2)	DDS···DDS	8.74	1.7	–3.2	–10.8	4.4	–7.2
11 (2)	DDS···CTC	7.81	–1.6	–0.6	–8.2	6.4	–5.3
12 (2)	CTC···CTC	5.79	–1.5	–0.1	–6.9	6.7	–3.5
13 (2)	DDS···DDS	10.51	1	–1.1	–5.1	1.6	–3.2
14 (2)	DDS···CTC	10.24	1	–0.2	–3	1.2	–1
S-ACO (#110_RT), $E_{cluster}$ = –221.3 kJ mol^{-1}							
1 (1)	DDS···DDS	7.21	–18.4	–7.5	–27	12	–41.1
2 (2)	DDS···DDS	8.26	–32.7	–8.2	–12.7	28.8	–33.9
3 (2)	DDS···ACO	3.99	–9.8	–2.2	–32.1	20.9	–27
4 (2)	DDS···ACO	7.8	–28.6	–6	–7.7	24.5	–26.4
5 (2)	DDS···DDS	11.67	–22.4	–5	–12.8	22.3	–24.7
6 (2)	DDS···ACO	6	–12.1	–2	–15.5	9.7	–21.7
7 (2)	DDS···DDS	8.33	–15.7	–4.8	–9.5	11.4	–21.4
8 (2)	DDS···DDS	5.98	2	–5.2	–25.1	14.2	–14.8
9 (1)	DDS···DDS	9.60	–8.1	–0.8	–4.1	0.4	–12.5
10 (2)	DDS···DDS	11.54	–2.9	–1.4	–6.1	1.1	–8.8
11 (2)	DDS···ACO	5.89	0.6	–0.7	–10	3.2	–6.7
12 (2)	ACO···ACO	5.98	–3.5	–1	–2.6	1.5	–5.8
13 (1)	ACO···ACO	6.40	–0.9	–0.2	–4.4	3	–3.1
14 (2)	DDS···ACO	9.17	1.1	–0.5	–4.6	2.5	–1.7
S-CHOX (#17_RT), $E_{cluster}$ = –238.6 kJ mol^{-1}							
1 (2)	DDS···DDS	8.24	–36.5	–9.3	–12.7	35.5	–34.6
2 (1)	DDS···DDS	7.77	–12.2	–4.4	–22.3	5.6	–32.1
3 (2)	DDS···CHOX	4.62	–8.7	–2.1	–40.6	28.7	–28.4
4 (2)	DDS···CHOX	8.56	–32.9	–8.5	–8.3	33.1	–27.8
5 (2)	DDS···DDS	11.77	–20	–4.1	–11.5	16.9	–23.7
6 (2)	DDS···CHOX	6	–9.4	–3	–22.2	16.8	–21.1
7 (1)	CHOX···CHOX	5.60	–10.1	–2.4	–9.3	2.8	–18.8
8 (2)	DDS···DDS	8.68	–9.2	–3.1	–7.1	2.8	–16.5
9 (2)	DDS···CHOX	6.58	–5.8	–2	–11.9	3.3	–16
10 (2)	DDS···DDS	6.07	5.3	–4.3	–23.6	11.5	–11
11 (1)	DDS···DDS	10.15	–7.2	–0.6	–2.8	0.1	–10.4
12 (2)	DDS···DDS	11.83	–4.1	–1.5	–6.7	1.8	–10.1
13 (2)	DDS···CHOX	6.59	–1	–0.4	–10.6	3.1	–8.7
14 (1)	CHOX···CHOX	6.68	–4.4	–1.1	–4.6	1.4	–8.6
15 (2)	CHOX···CHOX	6.07	0.6	–0.3	–12.7	8.1	–5.7

Inter-action	Molecules Involved	Distance (Å)	E_E (kJ mol^{-1})	E_P (kJ mol^{-1})	E_D (kJ mol^{-1})	E_R (kJ mol^{-1})	E_{tot}[b] (kJ mol^{-1})
S-DMF (#3), $E_{cluster}$ = –239.7 kJ mol^{-1}							
1 (1)	DDS···DDS	7.20	–15.5	–7.1	–31.4	16.2	–39.1
2 (2)	DDS···DDS	8.24	–35.2	–8.9	–12.8	33.2	–34.4
3 (2)	DDS···DMF	7.95	–34.5	–7.9	–8.3	30.8	–30.5
4 (2)	DDS···DMF	3.97	–8.7	–3.1	–34	19.2	–29.2
5 (2)	DDS···DMF	5.98	–12.5	–2.1	–16.7	6.7	–25.2
6 (2)	DDS···DDS	11.59	–23.1	–4.9	–13.5	24.2	–24.9
7 (2)	DDS···DDS	8.26	–16.7	–5.4	–10.5	14.7	–21.8
8 (1)	DMF···DMF	5.51	–8	–2.1	–4.6	1.7	–13
9 (2)	DDS···DDS	6.1	3.4	–4.8	–22.5	10.7	–12.9
10 (1)	DDS···DDS	9.71	–8.2	–0.9	–4.3	0.4	–12.8
11 (2)	DDS···DDS	11.37	–4.8	–1.5	–7.5	2.2	–11.3
12 (2)	DMF···DMF	6.1	–4.8	–2.4	–5.4	4.2	–9
13 (2)	DDS···DMF	6.42	0.5	–0.9	–10.7	4.3	–6.7
14 (1)	DMF···DMF	7.01	–0.6	–0.2	–3.2	0.5	–3.3
15 (2)	DDS···DMF	9.69	2.2	–0.5	–2.1	0.3	0.3
S-THF (#1941), $E_{cluster}$ = –225.8 kJ mol^{-1}							
1 (1)	DDS···DDS	7.00	–17.1	–8.4	–33.3	20.1	–40.8
2 (2)	DDS···DDS	8.54	–30.1	–7.7	–11.3	24.5	–32.2
3 (2)	DDS···THF	7.73	–27.6	–6.2	–11	24	–28.5
4 (2)	DDS···DDS	11.6	–23	–4.8	–13.1	22.4	–25.4
5 (2)	DDS···THF	4.1	–7.6	–1.6	–33.5	21.1	–25.2
6 (2)	DDS···DDS	8.73	–18.8	–5.2	–9	15.6	–22
7 (2)	DDS···THF	6.38	–7.8	–1.6	–15.1	7.2	–18.1
8 (2)	DDS···DDS	5.9	2.3	–5.4	–26.6	15.7	–15
9 (1)	DDS···DDS	9.20	–9.5	–1	–5.1	0.7	–14.8
10 (2)	DDS···DDS	11.7	–3.5	–1.4	–6.5	1.4	–9.5
11 (2)	DDS···THF	5.98	–1.3	–0.3	–12.9	5.6	–9.4
12 (1)	THF···THF	5.70	–2.6	–0.6	–3.9	0.7	–6.2
13 (1)	THF···THF	6.03	–0.4	–0.1	–6.8	1.9	–5.2
14 (2)	THF···THF	5.9	–1.5	–0.4	–5.5	3.3	–4.6
15 (2)	DDS···THF	8.92	0.2	-0.4	-3.4	1.1	-2.4
S-MEK (#62[1]), $E_{cluster}$ = –201.8 kJ mol^{-1}							
1 (2)	DDS···DDS	9.88	–31.2	–7.6	–9.5	24.1	–32
2 (2)	DDS···DDS	8.61	–24.5	–6.7	–13.6	18.5	–31.4
3 (2)	DDS···DDS	9.58	–31.7	–8.2	–8.2	25	–31.2
4 (2)	DDS···MEK	8.53	–29.6	–7.6	–11.3	30.8	–27.7
5 (2)	DDS···MEK	3.79	–3.8	–2.6	–29	15.5	–21.5
6 (2)	DDS···MEK	6.06	–2.7	–2.4	–16.3	7.1	–14.4
7 (1)	DDS···DDS	10.62	–7	–1	–9.3	4.2	–13.7
8 (2)	DDS···DDS	6.48	5.3	–5	–23	10	–12
9 (2)	DDS···MEK	7.81	–1.6	–1	–6.6	4.5	–5.5
10 (1)	DDS···DDS	7.78	–0.3	–0.5	–5.2	0.2	–5.1
11 (2)	MEK···MEK	5.97	–1.1	–0.8	–5.1	1.8	–5
12 (2)	DDS···MEK	7.97	–0.4	–0.7	–8	5.4	–4.5
13 (2)	DDS···MEK	6.92	0.7	–1.6	–10	8.8	–3.7
14 (2)	DDS···MEK	7.99	–0.9	–0.2	–1.9	0.2	–2.7
15 (2)	DDS···DDS	8.71	5.5	–1.7	–9	4.1	–0.8

Inter-action	Molecules Involved	Distance (Å)	E_E (kJ mol^{-1})	E_P (kJ mol^{-1})	E_D (kJ mol^{-1})	E_R (kJ mol^{-1})	E_{tot}[b] (kJ mol^{-1})
S-DCE (#713[1]), $E_{cluster}$ = –197.5 kJ mol^{-1}							
1 (2)	DDS···DDS	9.63	–28.3	–7.5	–8.9	21.1	–30.1
2 (1)	DDS···DCE	4.07	–12.7	–3.7	–30.4	22.1	–29
3 (2)	DDS···DDS	10.04	–22.3	–5.4	–8.7	10.1	–28.9
4 (2)	DDS···DDS	8.68	–21.3	–6.7	–13.1	17	–28.4
5 (2)	DDS···DDS	9.42	–6.9	–2.2	–9.1	3.7	–14.6
6 (2)	DDS···DDS	6.32	3.3	–5.6	–28.4	17.5	–14.5
7 (2)	DDS···DCE	7.7	–11.1	–2.2	–9.9	13	–14
8 (2)	DDS···DCE	7.71	–7.7	–1.2	–8.9	4.9	–13.7
9 (1)	DCE···DCE	6.13	–7.9	–0.9	–7.9	11.7	–8.6
10 (2)	DDS···DCE	5.74	0	–2.4	–18.3	15.4	–8.2
11 (2)	DDS···DCE	7.9	–8.6	–0.9	–6	14.2	–6.2
12 (2)	DDS···DCE	5.85	0.8	–0.6	–10.9	9.4	–3.3
13 (1)	DDS···DDS	8.00	1.3	–0.4	–3.8	0.1	–2.2
14 (2)	DDS···DDS	8.95	3.8	–1.2	–6.6	2.2	–1.2
S-DX (#207), $E_{cluster}$ = –232.8 kJ mol^{-1}							
1 (1)	DDS···DDS	7.75	–23.2	–6.2	–20.2	15.6	–37.1
2 (2)	DDS···DDS	8.59	–33.8	–9.7	–16.5	36	–35
3 (2)	DDS···DDS	9.08	–20	–5.2	–13.4	10.8	–30
4 (2)	DDS···DX	8.44	–29	–6.9	–12.1	33.1	–25.8
5 (2)	DDS···DDS	8.70	–14.6	–4.5	–15.5	11.3	–25.3
6 (2)	DDS···DX	3.99	–2.1	–2.4	–33.3	18.6	–21.5
7 (1)	DDS···DDS	10.43	–9.3	–1.8	–14.2	11.1	–16.7
8 (2)	DDS···DX	5.18	–6.4	–2	–19	14.2	–16
9 (2)	DDS···DX	7.7	–7.3	–2.7	–11.3	10	–13.4
10 (2)	DDS···DX	6.98	–4.1	–1.5	–15.2	8.7	–13.3
11 (2)	DDS···DDS	7.12	–1.9	–4.5	–9.4	2.9	–11.7
12 (2)	DDS···DX	7.57	–1.6	–0.9	–9.8	3.3	–8.9
13 (2)	DX···DX	5.81	–1	–0.1	–4.5	0.9	–4.5
14 (2)	DDS···DX	7.91	0.5	–1.4	–2.1	0.3	–2.2
15 (2)	DDS···DDS	13.32	5	–1.1	–3.6	0.6	1.7

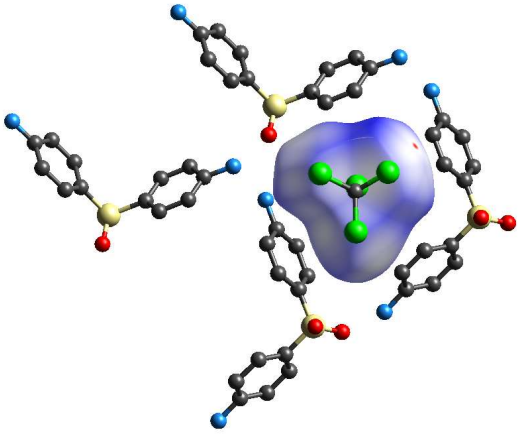
[a]Electrostatic (E_E), polarisation (E_P), dispersion (E_D) and exchange-repulsion energy (E_R) contributions. [b]$E_{tot} = k_E E_E + k_P E_P + k_D E_D + k_R E_R$, with k being scale factors.

Table S21. Overview (in %) of DDS···DDS, DDS···solvent and solvent···solvent intermolecular interactions seen in DDS monosolvate structures.

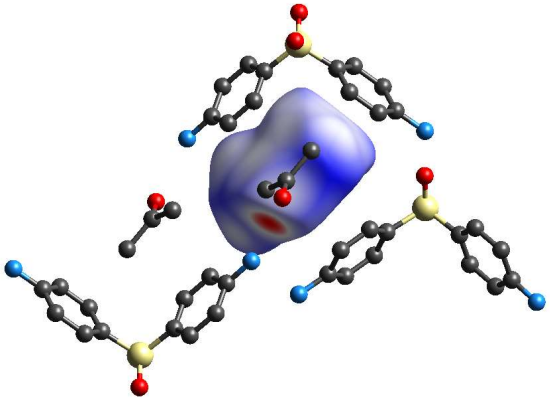
Solvate	$E_{cluster}$ / kJ mol^{-1}	E_{inter} (DDS···DDS) / %	E_{inter} (DDS···solvent) / %	E_{inter} (solvent···solvent) / %
S_{CTC}	–173.5	72.7	26.7	0.6
S_{ACO}	–221.3	58.9	37.7	3.3
S_{CHOX}	–238.6	49.1	42.8	8.1
S_{DMF}	–239.7	54.8	38.1	7.2
S_{THF}	–225.8	58.4	37.0	4.6
S_{MEK}	–201.8	57.9	39.6	2.5
S_{DCE}	–197.5	60.2	37.7	2.2
S_{DX}	–232.8	54.6	43.4	1.9

6. Hirshfeld Surface Calculations

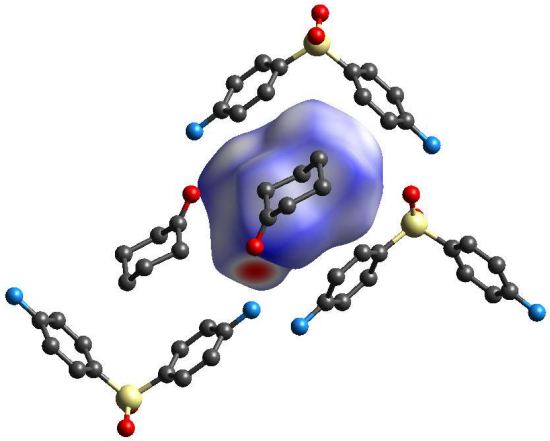
Hirshfeld d_{norm} plots for the solvent molecules in the solvate structures are shown in Figure S42.



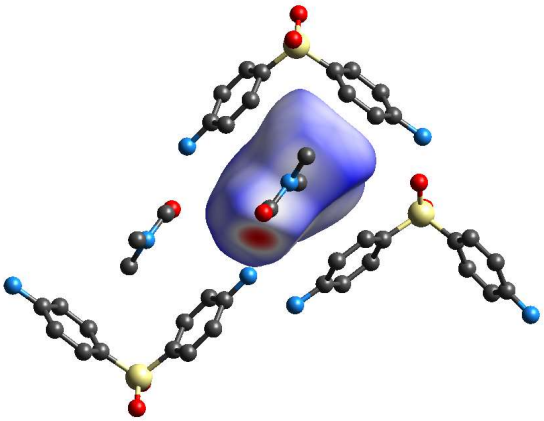
S$_{CTC}$: d_{norm} plot (mapped on the surface over the range –0.388 to 1.169 Å).



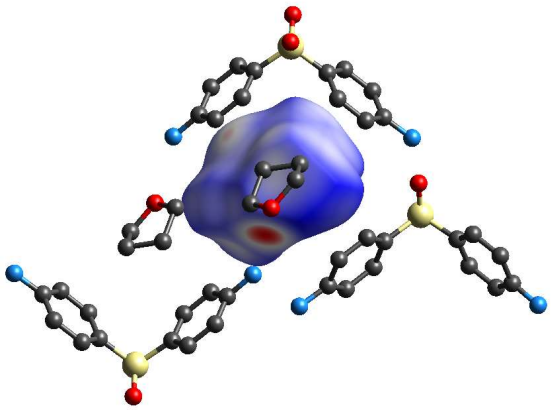
S$_{ACO}$: d_{norm} plot (mapped on the surface over the range –0.471 to 1.616 Å).



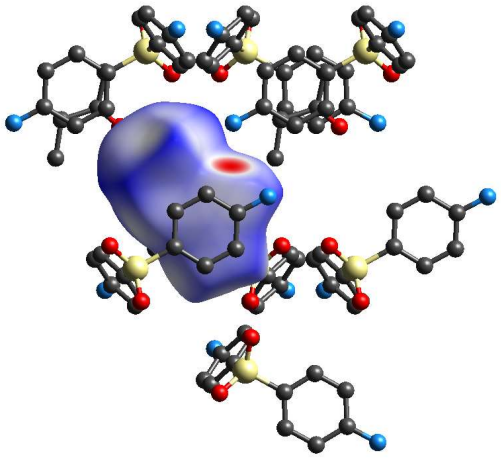
S$_{CHOX}$: d_{norm} plot (mapped on the surface over the range –0.524 to 1.479 Å).



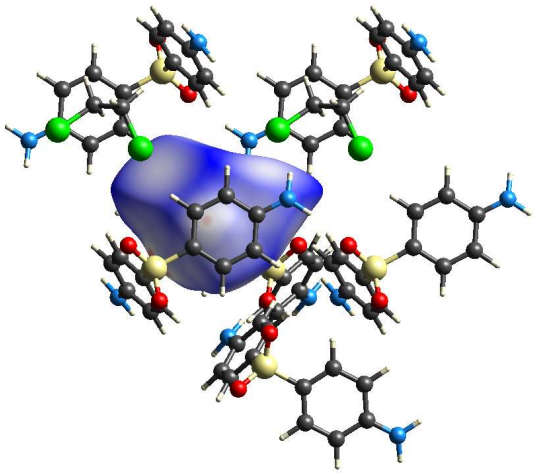
S$_{DMF}$: d_{norm} plot (mapped on the surface over the range –0.517 to 1.448 Å).



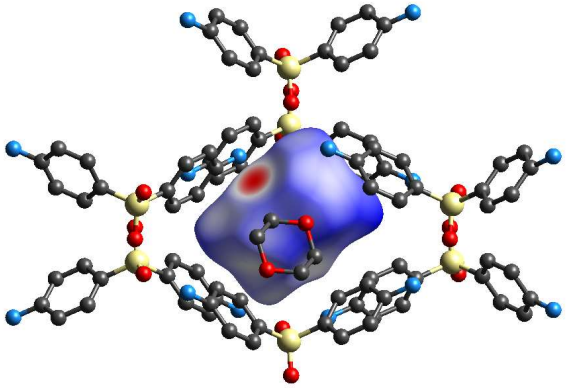
S$_{THF}$: d_{norm} plot (mapped on the surface over the range –0.445 to 1.356 Å).



S$_{MEK}$: d_{norm} plot (mapped on the surface over the range –0.508 to 1.455 Å).



S_{DCE}: d_{norm} plot (mapped on the surface over the range –0.506 to 1.416 Å).



S_{DX}: d_{norm} plot (mapped on the surface over the range –0.527 to 1.512 Å).

Figure S42. d_{norm} plots of the solvent molecules.

Table S22. Comparison of selected properties of the solvent molecules of the solvate structures.

	Volume / Å³	Area / Å²	Globularity	Asphericity	Strongest DDS···S Interaction / kJ mol⁻¹
III	290.92	269.80	0.787	0.144	
S_{CTC}	126.49	136.74	0.891	0.001	–14.5
S_{ACO}	97.37	113.29	0.903	0.037	–27.0
S_{CHOX}	146.07	150.08	0.894	0.035	–28.4
S_{DMF}	111.68	126.04	0.890	0.039	–30.5
S_{THF}	113.74	124.91	0.909	0.024	–28.5
S_{MEK}	125.23	137.43	0.881	0.079	–27.7
S_{DCE}	114.01	126.01	0.902	0.060	–29.0
S_{DX}	82.76	101.08	0.909	0.054	–25.8

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