Electronic Supplementary Material (ESI) for Soft Matter

Supporting information for

Application of solubility parameter in a D-Sorbitol-Based organogel in binary organic mixtures

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Table S1 Calculated Hansen solubility parameters and gelation behaviour for DCBS in binary organic mixed solvents [a].

Solvents	δ_d ($MPa^{1/2}$)	δ_p ($MPa^{1/2}$)	δ_h ($MPa^{1/2}$)	Gelation behaviour
Ethanol: Methylcyclohexane (v/v)				
90:10	15.82	7.92	17.56	S
80:20	15.84	7.04	15.72	S
70:30	15.86	6.16	13.88	PG
60:40	15.88	5.28	12.04	PG
50:50	15.9	4.4	10.2	G
40:60	15.92	3.52	8.36	G
30:70	15.94	2.64	6.52	G
20:80	15.96	1.76	4.68	G
10:90	15.98	0.88	2.84	P
05:95	15.99	0.44	1.92	P
Ethanol:n-Octane (v/v)				
90:10	15.77	7.92	17.46	S
80:20	15.74	7.04	15.52	S
70:30	15.71	6.16	13.58	PG

60:40	15.68	5.28	11.64	PG
50:50	15.65	4.4	9.7	G
40:60	15.62	3.52	7.76	G
30:70	15.59	2.64	5.82	G
20:80	15.56	1.76	3.88	G
10:90	15.53	0.88	1.94	P
05:95	15.52	0.44	0.97	P
Ethanol:n-Hexane (v/v)				
90:10	15.71	7.92	17.46	S
80:20	15.62	7.04	15.52	S
70:30	15.53	6.16	13.58	PG
60:40	15.44	5.28	11.64	G
50:50	15.35	4.4	9.7	G
40:60	15.26	3.52	7.76	G
30:70	15.17	2.64	5.82	G
20:80	15.08	1.76	3.88	P
10:90	14.99	0.88	1.94	P
05:95	14.95	0.44	0.97	P
Ethanol:Cyclohexane (v/v)				
90:10	15.9	7.92	17.48	S

80:20	16	7.04	15.56	S
70:30	16.1	6.16	13.64	S
60:40	16.2	5.28	11.72	PG
50:50	16.3	4.4	9.8	G
40:60	16.4	3.52	7.88	G
30:70	16.5	2.64	5.96	G
20:80	16.6	1.76	4.04	G
10:90	16.7	0.88	2.12	P
05:95	16.75	0.44	1.16	P
Ethanol:n-Octanol (v/v)				
90:10	15.92	8.25	18.65	S
80:20	16.04	7.7	17.9	S
70:30	16.16	7.15	17.15	S
60:40	16.28	6.6	16.4	S
50:50	16.4	6.05	15.65	S
40:60	16.52	5.5	14.9	G
30:70	16.64	4.95	14.15	G
20:80	16.76	4.4	13.4	G
10:90	16.88	3.85	12.65	G
Ethanol:Toluene (v/v)				
90:10	16.02	8.06	17.66	S

80:20	16.24	7.32	15.92	S
70:30	16.46	6.58	14.18	S
60:40	16.68	5.84	12.44	PG
50:50	16.9	5.1	10.7	G
40:60	17.12	4.36	8.96	G
30:70	17.34	3.62	7.22	G
20:80	17.56	2.88	5.48	G
10:90	17.78	2.14	3.74	G
Ethanol:Ethyl acetate (v/v)				
90:10	15.8	8.45	18.18	S
70:30	15.8	8.1	16.96	S
60:40	15.8	7.75	15.74	S
50:50	15.8	7.4	14.52	PG
30:70	15.8	7.05	13.3	G
20:80	15.8	6.7	12.08	G
10:90	15.8	6.35	10.86	G

[a]Concentration: 2% (w/v). S: solution, PG: partial gel, G: gel, P: precipitation.

Table S2 Summary of group additivity values for DCBS.

	Fedors Method[a]						
Groups	$-CH_2$	$-CH<$	−Cl (Halogen attached to carbon atom with double bond)	−OH (disubstituted or on adjacent C)	−O−	Ring closure 5 or more atoms	Phenyl (trisubstituted)
Occurrences, N_i	2	5	2	4	2	1	1
E_i (J/mol)	4940	3430	9240	21850	3350	1050	31940
V_i (cm^3/mol)	16.1	-1.0	4.0	13.0	3.8	16.0	33.4
Sum		$E_{coh} = \sum E_i N_i = 172600$ $V = \sum V_i N_i = 144.2$					
δ ($J^{1/2}/cm^{3/2}$)		$\delta = (E_{coh}/V)^{1/2} = 34.60$					

[a]All this data was taken from Van Krevelen, D. W. H. P. J. Properties of Polymers. Elsevier Scientific Publishing: New York, 1976.

Table S3 Calculated Flory-Huggins parameter (χ) of DCBS in ethanol-methylcyclohexane mixtures for an example.

Example: Estimation of the Flory-Huggins parameter (χ) of DCBS gelator in 50% methylcyclohexane volume fraction in ethanol-methylcyclohexane mixtures.
Solution: The Hildebrand solubility parameter $\delta=\delta_{C2H5OH}$* vol fraction+δ_{C7H14}* (1-vol fraction) =26*0.5+16*0.5=21.0 $J^{1/2}/cm^{3/2}$ The molar volume $V=V_{C2H5OH}$* vol fraction+V_{C7H14}* (1-vol fraction) =58.5*0.5+128.3*0.5=80.4cm^3/mol According to eq $\chi=V_1(\delta_2-\delta_1)^2/RT=80.4*(34.60-21.0)^2/8.314/298.15=6.00$

Table S4 Calculated solubility parameters (δ), molar volume (V) and Flory-Huggins parameter (χ) for DCBS in various solvents[a].

Solvents	δ ($J^{1/2}/cm^{3/2}$)	V (cm^3/mol)	χ	Gelation behaviour
DCBS	34.6			
Methylcyclohexane	16.0	128.3	17.91	P
Cyclohexane	16.8	108.7	13.89	P
n-Hexane	14.9	131.6	20.6	P

n-Octane	15.5	163.5	24.06	P
Carbon tetrachloride	17.6	97.1	11.32	P
Toluene	18.2	106.8	11.59	G
n-Octanol	21.1	157.7	11.59	G
Ethyl acetate	18.6	98.5	10.17	G
n-Butanol	23.3	91.5	4.71	G
Ethanol	26.0	58.5	1.75	S
Ethanol: Methylcyclohexane (v/v)				
90:10	25	61.87	2.30	S
80:20	24	65.64	2.98	S
70:30	23	69.91	3.79	S
60:40	22	74.77	4.79	PG
50:50	21	80.36	6.00	G
40:60	20	86.85	7.47	G
30:70	19	94.48	9.28	G
20:80	18	103.58	11.51	G
10:90	17	114.62	14.32	P
05:95	16.5	121.08	16.00	P
Ethanol:n-Octane (v/v)				
90:10	24.95	62.51	2.35	S

80:20	23.9	67.12	3.10	S
70:30	22.85	72.46	4.04	PG
60:40	21.8	78.72	5.20	PG
50:50	20.75	86.17	6.67	G
40:60	19.7	95.17	8.52	G
30:70	18.65	106.28	10.91	G
20:80	17.6	120.31	14.03	G
10:90	16.55	138.62	18.22	P
05:95	16.03	150.04	20.87	P
Ethanol:n-Hexane (v/v)				
90:10	24.89	61.94	2.36	S
80:20	23.78	65.81	3.11	S
70:30	22.67	70.20	4.03	PG
60:40	21.56	75.21	5.16	G
50:50	20.45	81.00	6.54	G
40:60	19.34	87.74	8.24	G
30:70	18.23	95.72	10.35	G
20:80	17.12	105.29	12.98	P
10:90	16.01	116.98	16.31	P
05:95	15.46	123.86	18.31	P
Ethanol:Cyclohexane (v/v)				

90:10	25.08	61.33	2.24	S
80:20	24.16	64.45	2.83	S
70:30	23.24	67.91	3.54	S
60:40	22.32	71.76	4.37	PG
50:50	21.4	76.06	5.35	G
40:60	20.48	80.92	6.51	G
30:70	19.56	86.45	7.89	G
20:80	18.64	92.78	9.53	G
10:90	17.72	100.11	11.51	P
05:95	17.26	104.23	12.64	P
Ethanol:n-Octanol (v/v)				
90:10	25.51	62.43	2.08	S
80:20	25.02	66.92	2.48	S
70:30	24.53	72.11	2.95	S
60:40	24.04	78.17	3.52	S
50:50	23.55	85.34	4.20	S
40:60	23.06	93.96	5.05	G
30:70	22.57	104.53	6.10	G
20:80	22.08	117.76	7.45	G
10:90	21.59	134.84	9.21	G
Ethanol:Toluene (v/v)				
90:10	25.22	61.27	2.17	S

80:20	24.44	64.32	2.68	S
70:30	23.66	67.68	3.27	S
60:40	22.88	71.42	3.96	PG
50:50	22.1	75.59	4.76	G
40:60	21.32	80.29	5.71	G
30:70	20.54	85.60	6.83	G
20:80	19.76	91.66	8.14	G
10:90	18.98	98.65	9.71	G
Ethanol:Ethyl acetate (v/v)				
90:10	25.26	60.98	2.15	S
70:30	23.78	66.62	3.15	S
60:40	23.04	69.85	3.77	S
50:50	22.3	73.40	4.48	PG
30:70	20.82	81.73	6.26	G
20:80	20.08	86.65	7.37	G
10:90	19.34	92.20	8.66	G
Concentration: 2% (w/v). S: solution, PG: partial gel, G: gel, P: precipitation.				

[a]One-component molar volume and solubility parameters are taken from reference 29.

The solubility parameter values of the mixed solvents were calculated using $\delta=\sum\varphi_i\delta_i$ (Equ. 68 of reference 29)

Table S5 Summarizes of the Flory-Huggins parameter (χ) for various mixed solvents to verify the model.

Solvents	δ ($J^{1/2}/cm^{3/2}$)	V (cm^3/mol)	χ	Gelation behaviour
Ethanol:Carbon tetrachloride (v/v=9:1)	25.16	60.92	2.19	S
Ethanol:Acetonitrile (v/v=5:5)	25.15	55.39	2.00	S
Ethanol:Carbon tetrachloride (v/v=3:7)	20.12	81.06	6.86	G
Ethanol:Benzene (v/v=3:7)	20.96	77.17	5.79	G

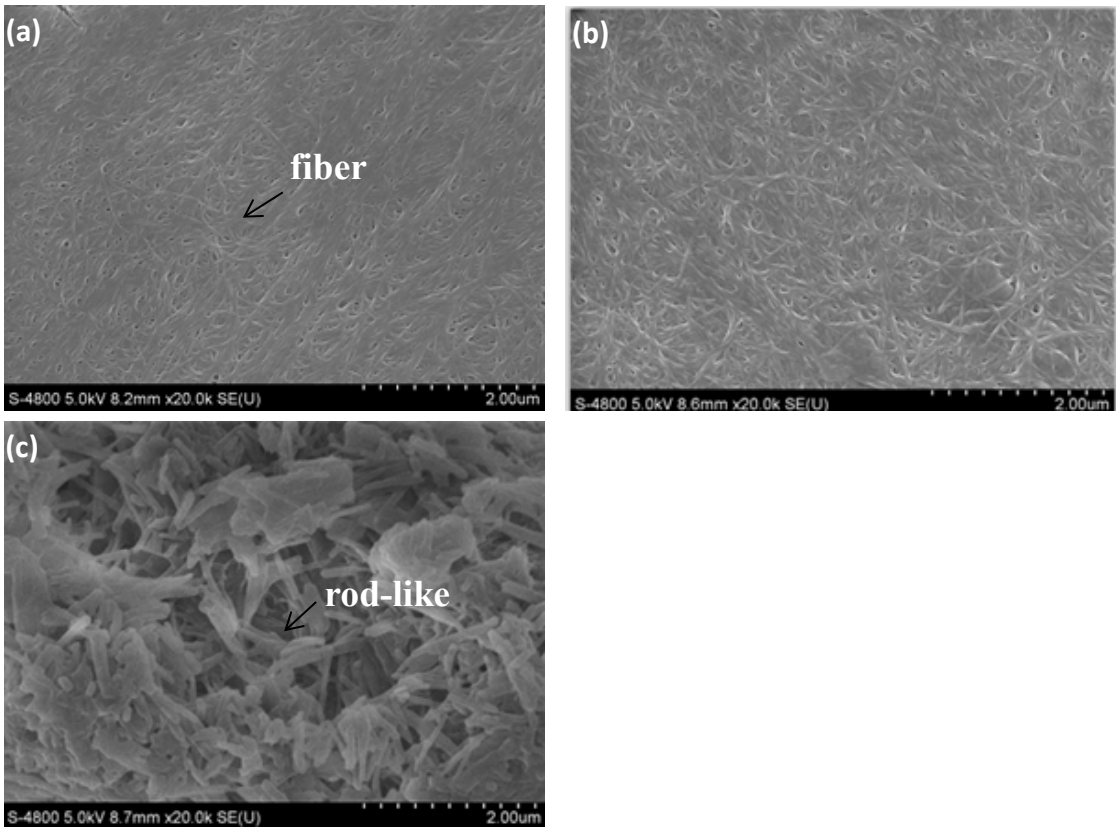

Fig. S1 SEM images of DCBS xerogels and precipitates (2% w/v) in different methylcyclohexane contents: (a) 70%; (b) 80%; (c) 100%.

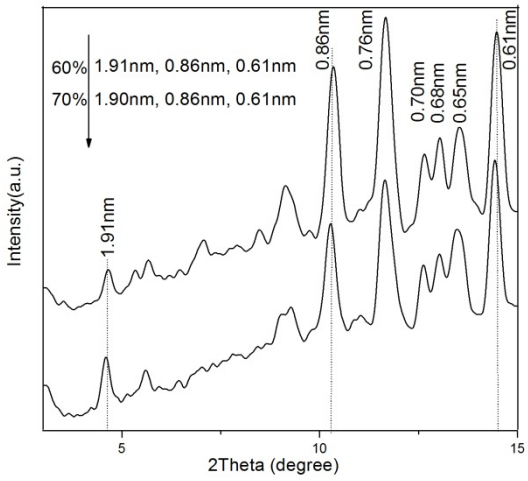

Fig. S2 XRD patterns of xerogels (2% w/v) at different methylcyclohexane contents: 60% and 70%.

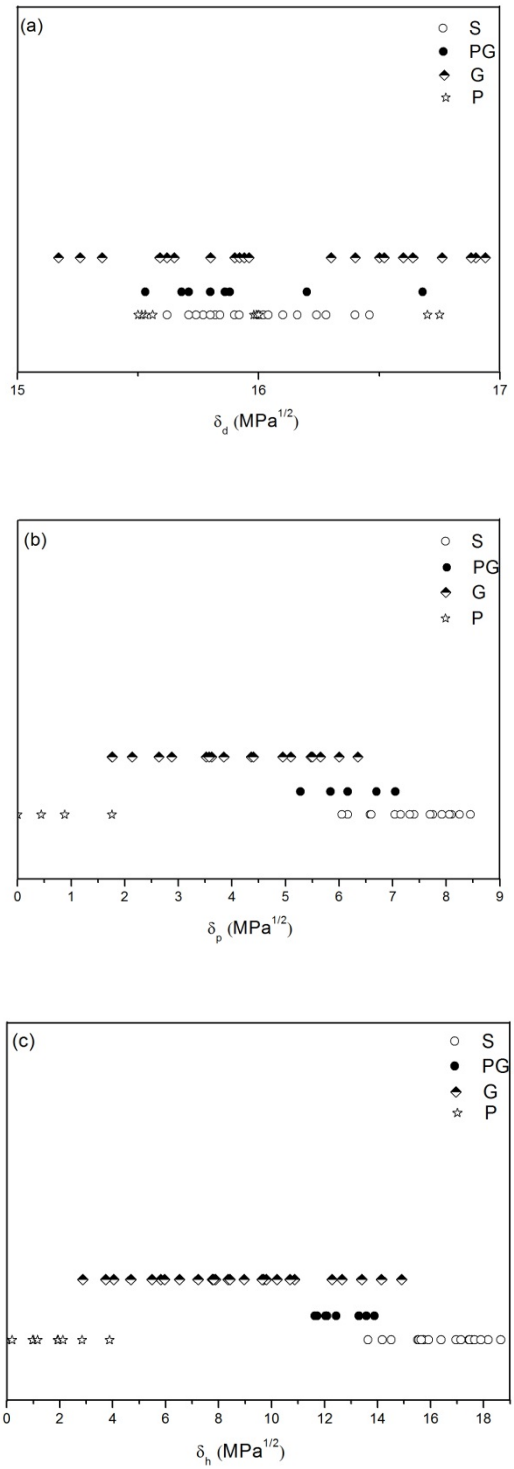

Fig. S3 Gelation behaviour of DCBS as a function of the Hansen parameters in the studied solvents: (a) δ_d, (b) δ_p, (c) δ_h.