

Organogel formation rationalized by Hansen solubility parameters: improved methodology

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Electronic supporting information

Table of contents:

1. Solubility results A5.....	S2
2. Comparison between NO method and AO method	S4
3. AO method applied to other studies	S14
4. NMR spectrum for LMWG A5	S27

1. Solubility results A5

Table S1 Gelation tests for LMWG **A5**, with pure liquids. ^{a-b}

Liquid	δ_d (MPa ^{1/2})	δ_p (MPa ^{1/2})	δ_h (MPa ^{1/2})	
acetonitrile	15.3	18	6.1	G
benzyl alcohol	18.4	6.3	13.7	S
1-butanol	16	5.7	15.8	S
t-butyl acetate	15	3.7	6	G
1-chloropentane	16	6.9	1.9	G
chlorobenzene	19	4.3	2	G
cyclohexane	16.8	0	0.2	G
cyclohexanone	17.8	8.4	5.1	S
diacetone alcohol	15.8	8.2	10.8	S
dimethylformamide (DMF)	17.4	13.7	11.3	S
dimethylsulfoxide (DMSO)	18.4	16.4	10.2	P
1,4-dioxane	17.5	1.8	9	S
ethanolamine	17	15.5	21	G
hexadecane	16.3	0	0	G
methanol	14.7	12.3	22.3	S
methylethylketone (MEK)	16	9	5.1	G
N,N-diethyl acetamide	16.4	11.3	7.5	S
propylene carbonate	20	18	4.1	G
propylene glycol	16.8	10.4	21.3	S
toluene	18	1.4	2	G
water	15.5	16	42.3	P
N-methylformamide	17.4	18.8	15.9	S

^a Gelation is tested by introducing 10 mg of gelator and 1 mL of liquid in a screw-cap vial, heating until dissolution and leaving the vial to cool on the bench.

^b G: gel; S: soluble; P: insoluble or formation of a precipitate after cooling.

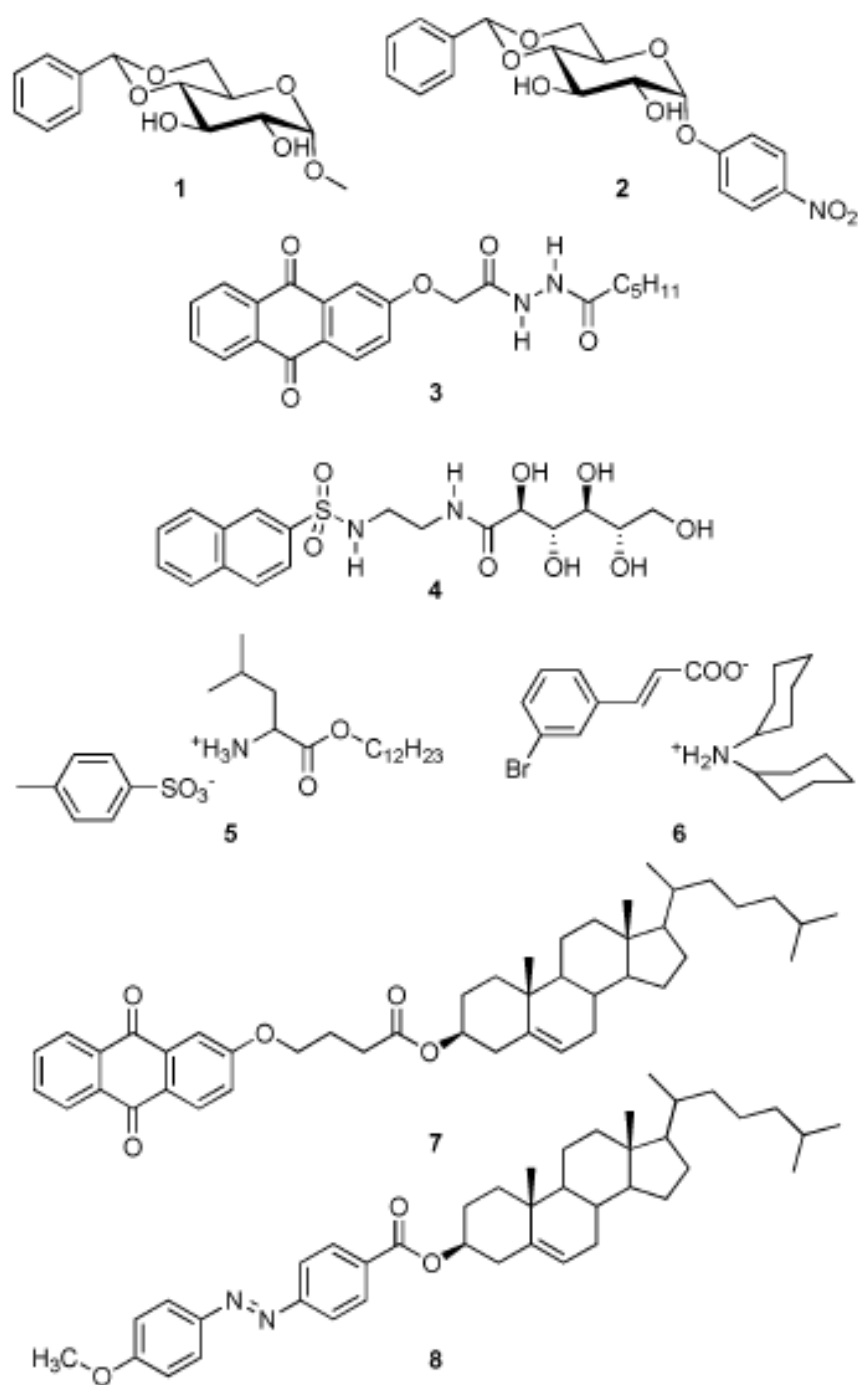
Table S2 Gelation tests for LMWG **A5**, with mixtures of liquids.^{a-b}

Liquid 1	Liquid 2	Composition (%)	δ_d (MPa ^{1/2})	δ_p (MPa ^{1/2})	δ_h (MPa ^{1/2})	
dimethylformamide (DMF)	methanol	0/100	14.7	12.3	22.3	S
		25/75	15.37	12.65	19.55	S
		50/50	16.05	13	16.8	S
		75/25	16.72	13.6	14.05	S
		100/0	17.4	13.7	11.3	S
methanol	water	0/100	15.5	16	42.3	P
		25/75	15.3	15.07	37.3	P
		50/50	15.1	14.15	32.3	G
		75/25	14.9	13.22	27.3	G
		100/0	14.7	12.3	22.3	S
cyclohexanone	acetonitrile	0/100	15.3	18	6.1	G
		25/75	15.92	15.6	5.85	G
		50/50	16.55	13.2	5.6	S
		75/25	17.17	10.8	5.35	S
		100/0	17.8	8.4	5.1	S
diacetone alcohol	1,4-dioxane	0/100	17.5	1.8	9	S
		25/75	17.07	3.4	9.45	S
		50/50	16.65	5	9.9	S
		75/25	16.22	6.6	10.35	S
		100/0	15.8	8.2	10.8	S
water	N-methylformamide	0/100	17.4	18.8	15.9	S
		25/75	16.92	18.1	22.5	G
		50/50	16.45	17.4	29.1	G
		75/25	15.97	16.7	34.95	P
		100/0	15.5	16	42.3	P

^a Gelation is tested by introducing 10 mg of gelator and 1 mL of liquid in a screw-cap vial, heating until dissolution and leaving the vial to cool on the bench.

^b G: gel; S: soluble; P: insoluble or formation of a precipitate after cooling.

2. Comparison between NO method and AO method



Scheme 1

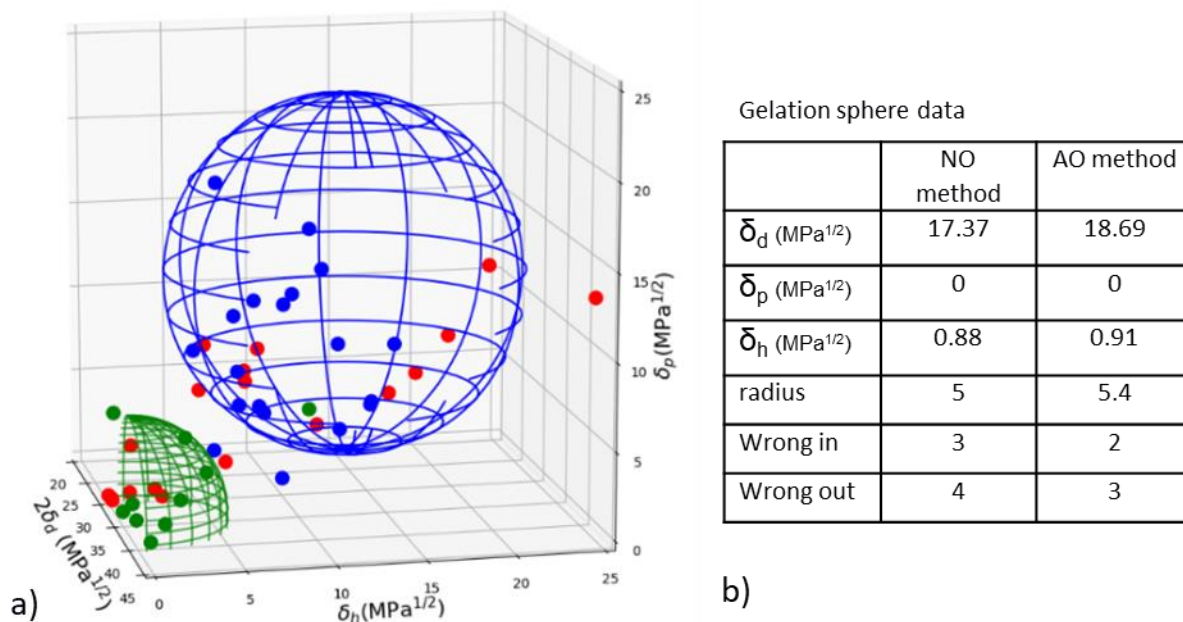


Figure S1. (a) Solubility data for LMWG 1 (scheme 1) represented in Hansen space (data taken from reference¹ and previously treated with the NO method²). Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software [$\bar{\delta}_d = 18.85$; $\bar{\delta}_p = 14.17$; $\bar{\delta}_h = 12.05$; $R_{Sol} = 10.3$ MPa^{1/2}] and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵ software. (b) Centre, radius and outliers of the gelation sphere from the NO method and the AO method.

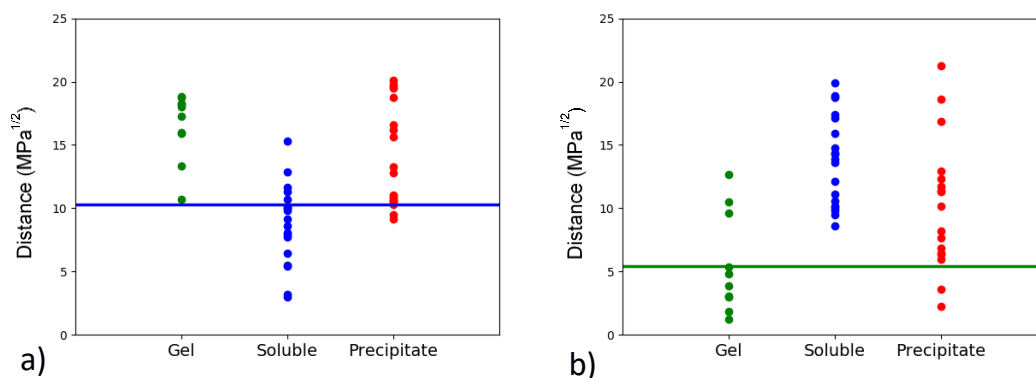


Figure S2. Distances in Hansen space to the centre of the solubility sphere (a) or to the centre of the gelation sphere (b) for LMWG 1 (AO method). The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble.

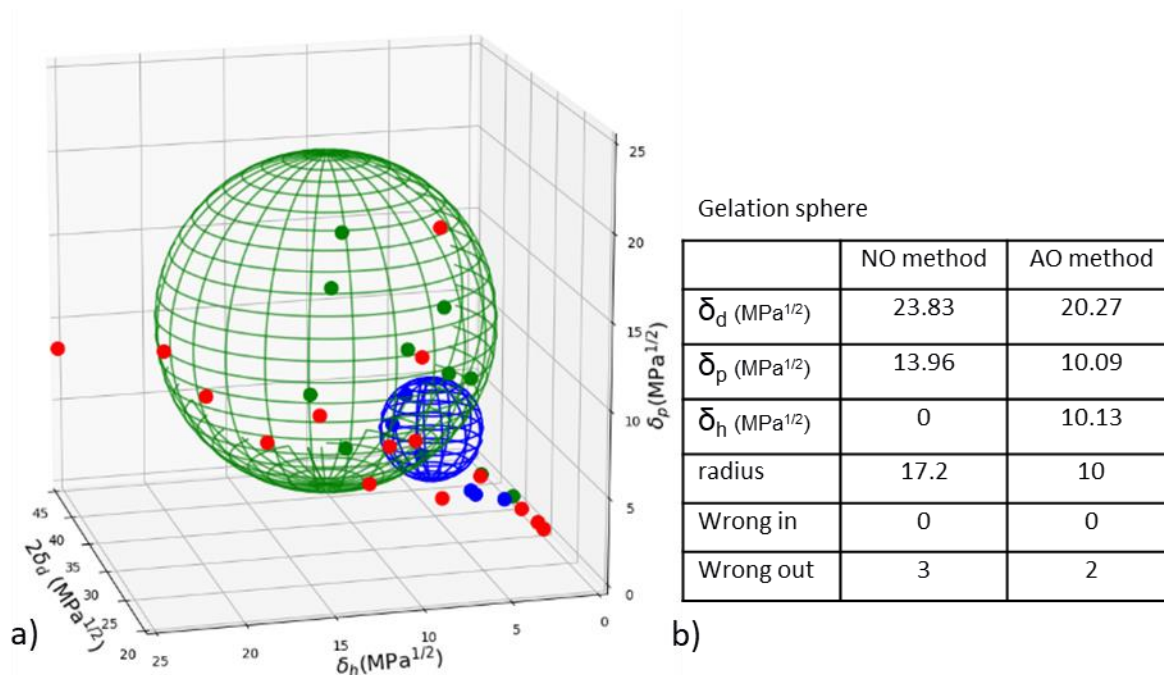


Figure S3. (a) Solubility data for LMWG 2 (scheme 1) represented in Hansen space (data taken from reference ⁶ and previously treated with the NO method²). Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software [$\bar{\delta}_d = 17.31$; $\bar{\delta}_p = 4.9$; $\bar{\delta}_h = 5.37$; $R_{Sol} = 3.0$ MPa^{1/2}] and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵ software. (b) Centre, radius and outliers of the gelation sphere from the NO method and the AO method.

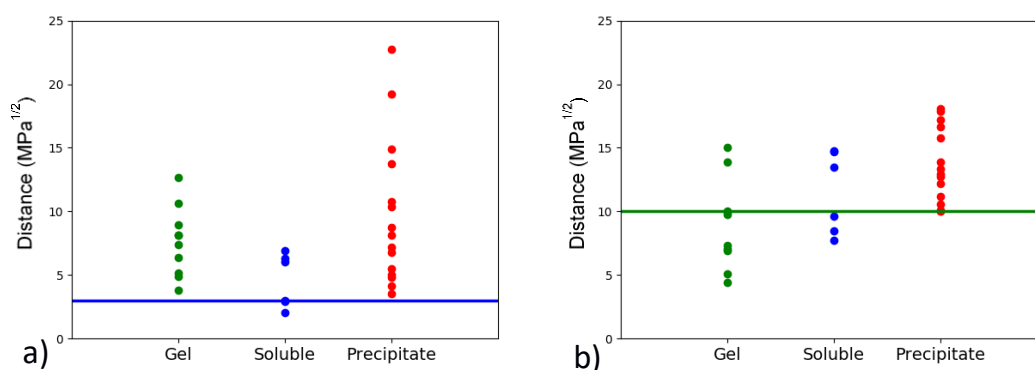


Figure S4. Distances in Hansen space to the centre of the solubility sphere (a) or to the centre of the gelation sphere (b) for LMWG 2 (AO method). The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble.

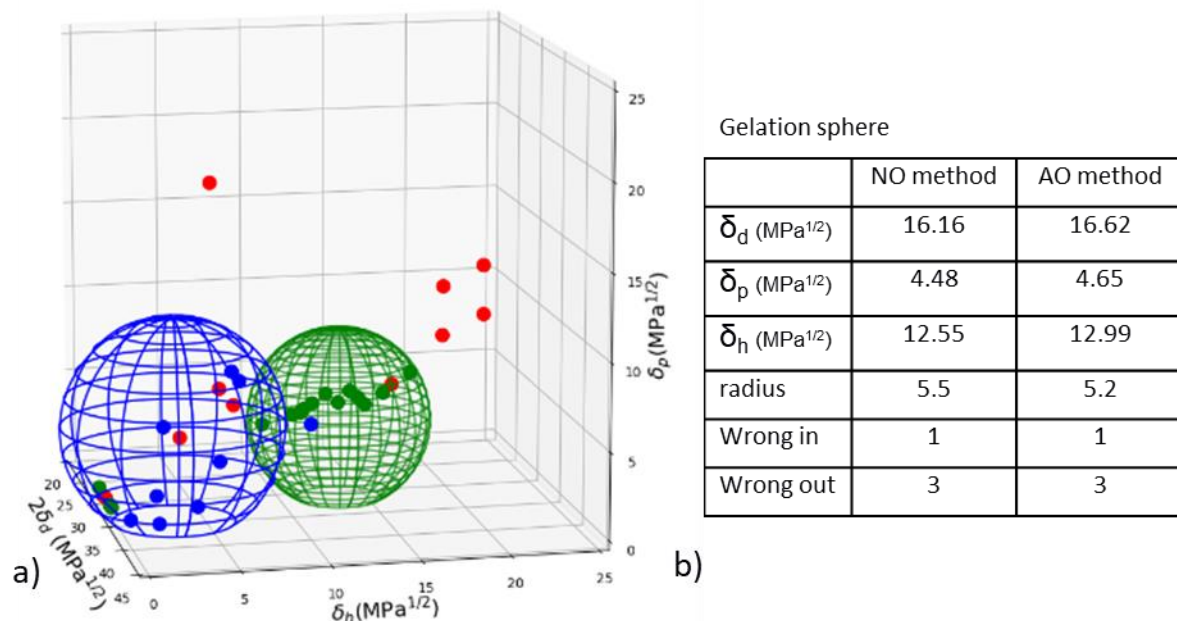


Figure S5. (a) Solubility data for LMWG 3 (scheme 1) represented in Hansen space (data taken from reference⁷ and previously treated with the NO method²). Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software [$\bar{\delta}_d = 18.31$; $\bar{\delta}_p = 5.36$; $\bar{\delta}_h = 2.9$; $R_{Sol} = 6.3$ MPa^{1/2}] and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵ software. **(b)** Centre, radius and outliers of the gelation sphere from the NO method and the AO method.

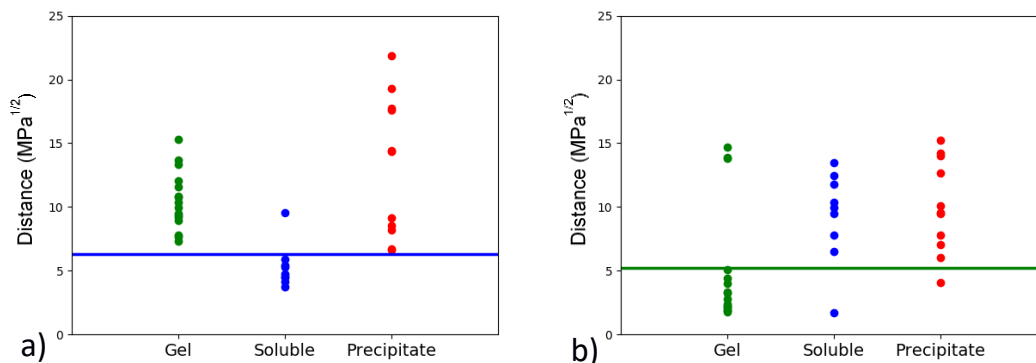


Figure S6. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG 3 (AO method). The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble.

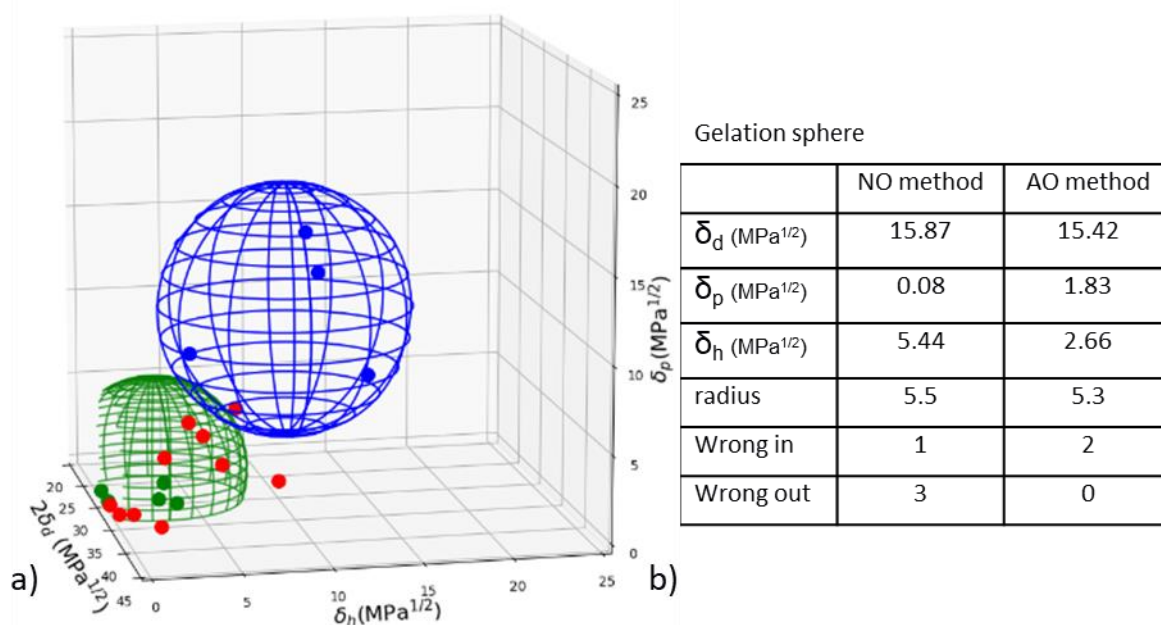


Figure S7. (a) Solubility data for LMWG 4 (scheme 1) represented in Hansen space (data taken from reference⁸ and previously treated with the NO method²). Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software [$\bar{\delta}_d = 18.29$; $\bar{\delta}_p = 12.05$; $\bar{\delta}_h = 9.11$; $R_{Sol} = 7.1$ MPa^{1/2}] and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵ software. **(b)** Centre, radius and outliers of the gelation sphere from the NO method and the AO method.

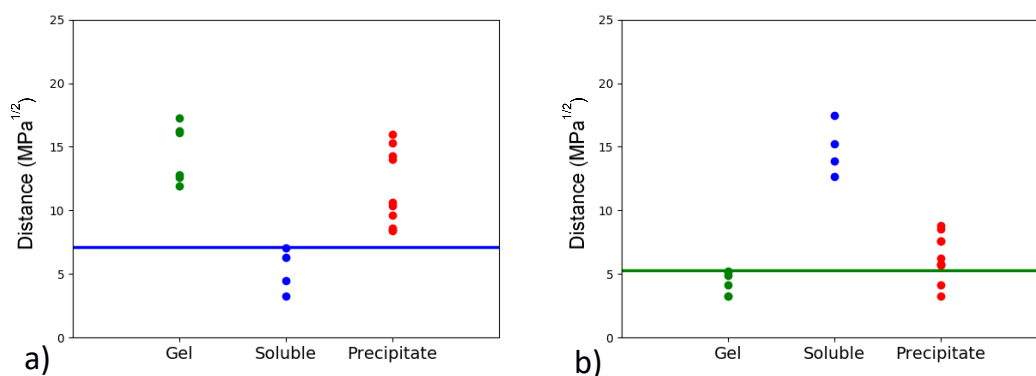


Figure S8. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG 4 (AO method). The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble.

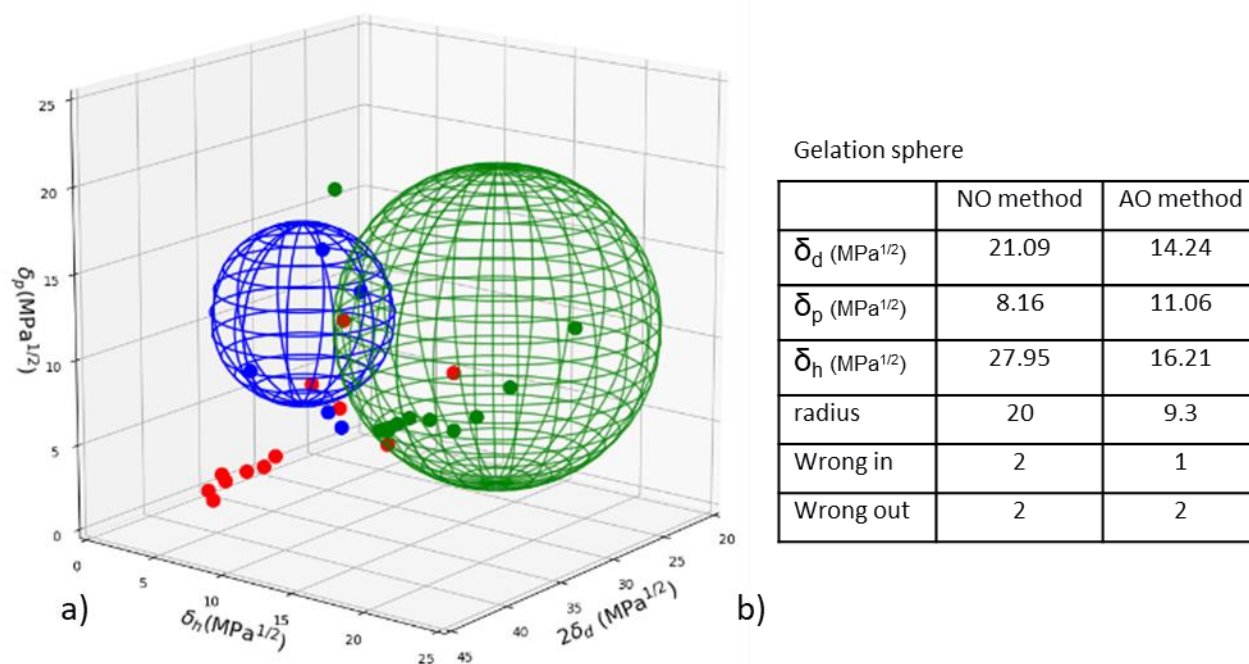


Figure S9. (a) Solubility data for LMWG 5 (scheme 1) represented in Hansen space (data taken from reference⁹ and previously treated with the NO method²). Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software [$\bar{\delta}_d = 18.65$; $\bar{\delta}_p = 12.56$; $\bar{\delta}_h = 9.18$; $R_{Sol} = 5.2$ MPa^{1/2}] and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵ software. **(b)** Centre, radius and outliers of the gelation sphere from the NO method and the AO method.

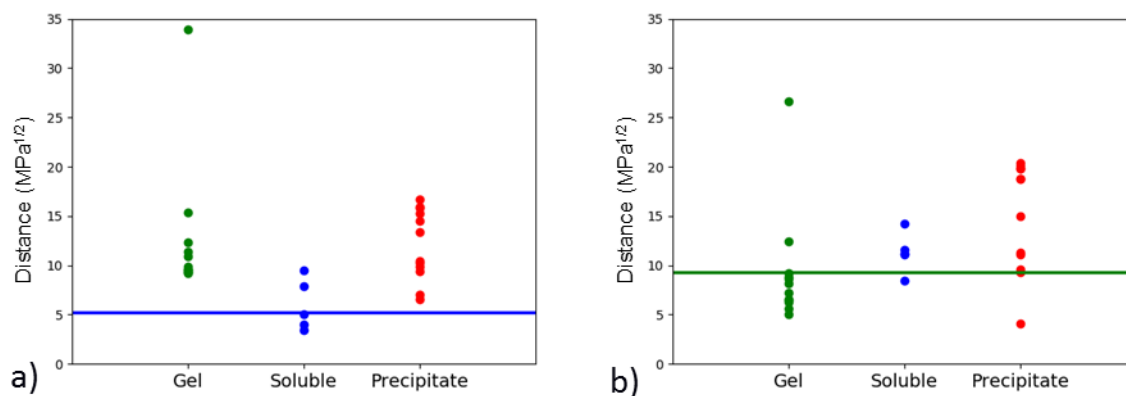


Figure S10. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG 5 (AO method). The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble.

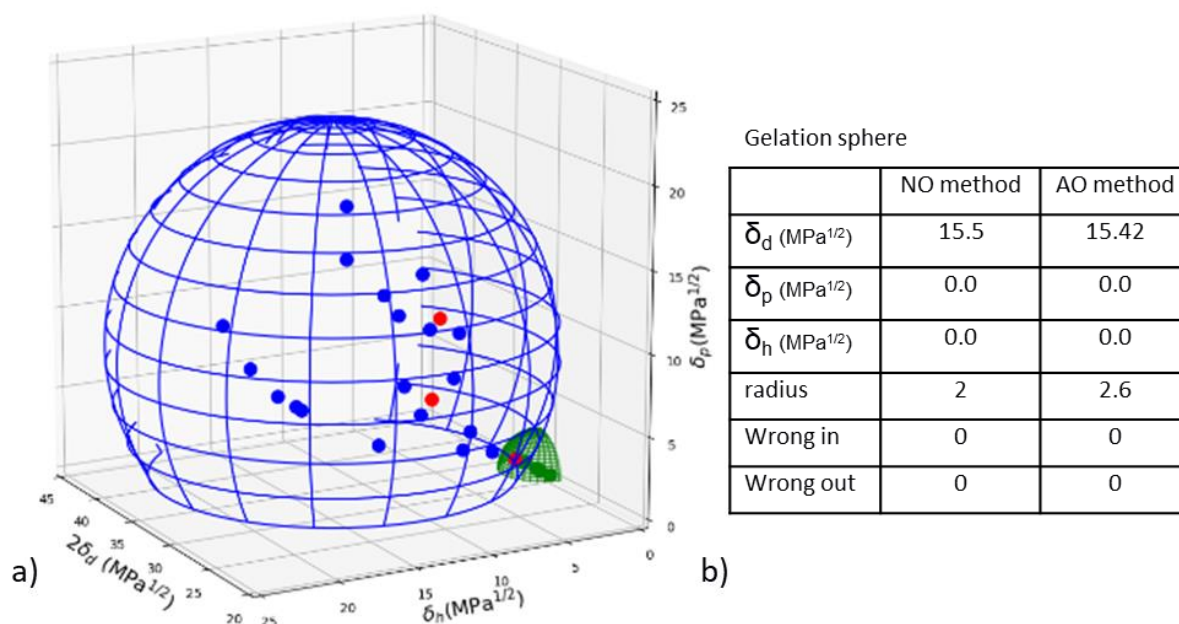


Figure S11. (a) Solubility data for LMWG 6 (scheme 1) represented in Hansen space (data taken from reference¹⁰ and previously treated with the NO method²). Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software [$\bar{\delta}_d = 18.09$; $\bar{\delta}_p = 8.11$; $\bar{\delta}_h = 11.45$; $R_{sol} = 13.7$ MPa^{1/2}] and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵ software. (b) Centre, radius and outliers of the gelation sphere from the NO method and the AO method.

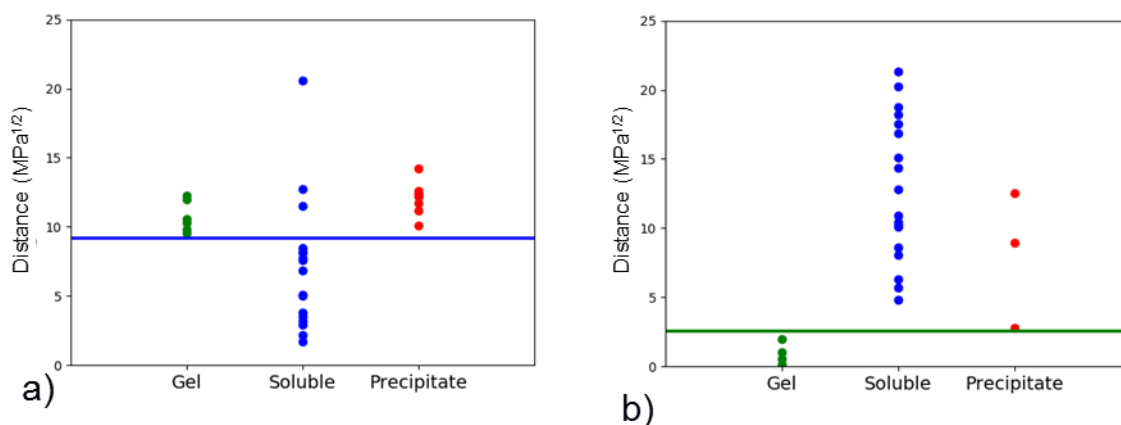


Figure S12. Distances in Hansen space to the centre of the solubility sphere (a) or to the centre of the gelation sphere (b) for LMWG 6 (AO method). The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble.

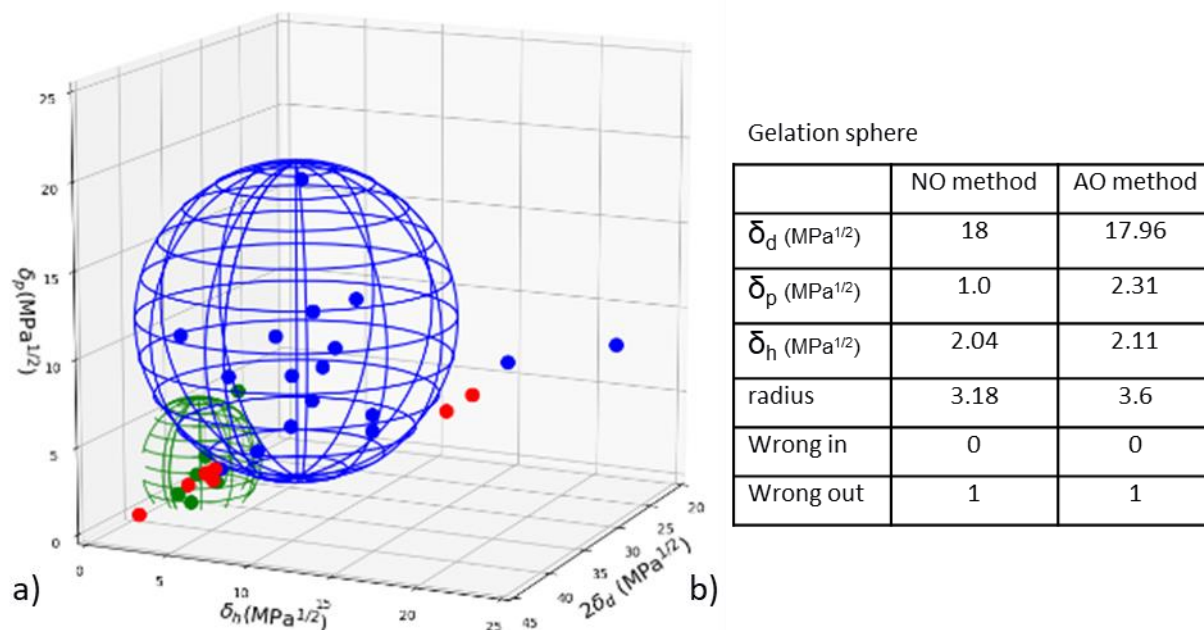


Figure S13. (a) Solubility data for LMWG 7 (scheme 1) represented in Hansen space (data taken from reference¹¹ and previously treated with the NO method²). Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software [$\bar{\delta}_d = 16.34$; $\bar{\delta}_p = 10.18$; $\bar{\delta}_h = 6.78$; $R_{Sol} = 9.2$ MPa^{1/2}] and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵ software. (b) Centre, radius and outliers of the gelation sphere from the NO method and the AO method.

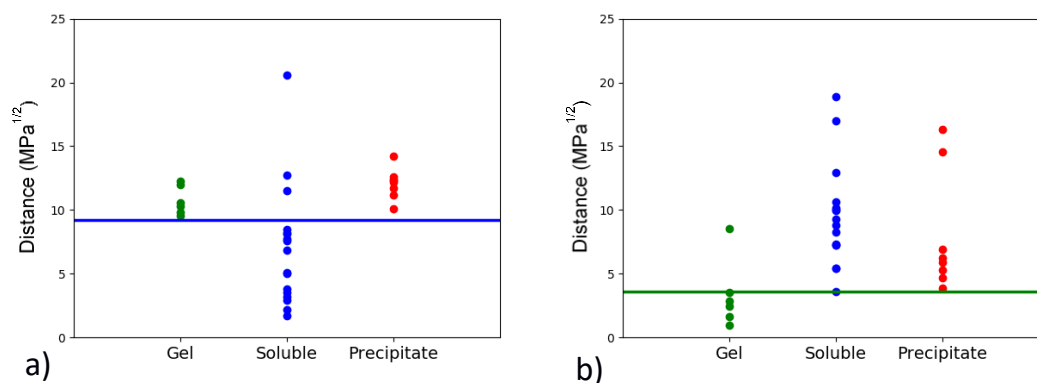


Figure S14. Distances in Hansen space to the centre of the solubility sphere (a) or to the centre of the gelation sphere (b) for LMWG 7 (AO method). The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble.

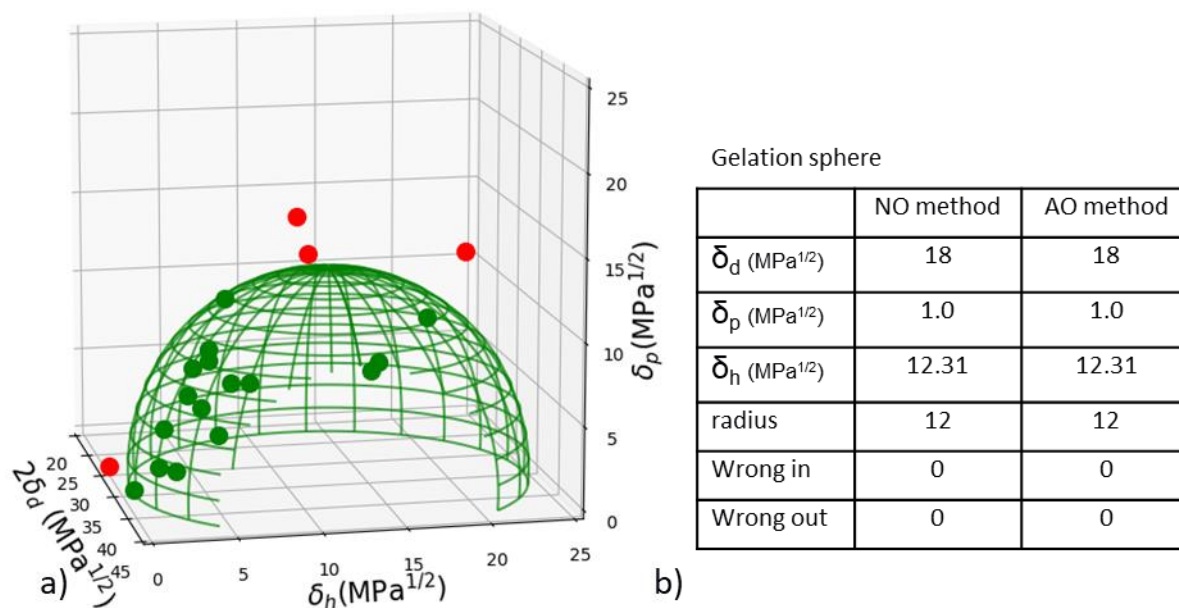


Figure S15. (a) Solubility data for LMWG **8** (scheme 1) represented in Hansen space (data taken from reference¹² and previously treated with the NO method²). Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. **(b)** Centre, radius and outliers of the gelation sphere from the NO method and the AO method. Both methods are identical since no **S** points are present in the data.

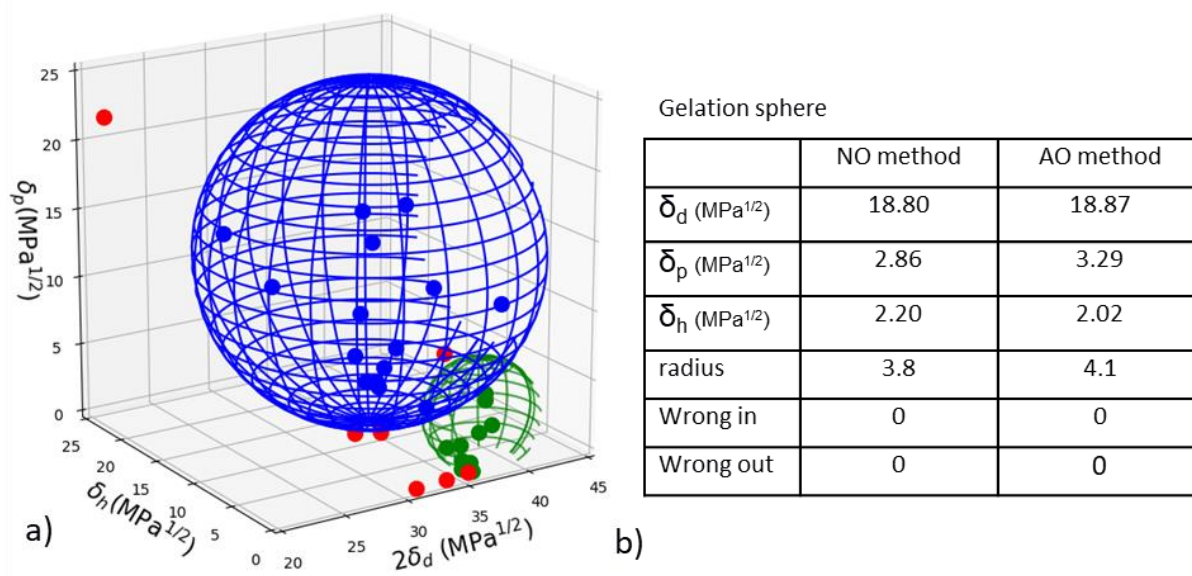


Figure S16. (a) Solubility data for LMWG **a1** reported by Brigitte Jamart-Grégoire et al.¹³ (previously treated with the NO method¹⁴) represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software [$\delta_d = 17.70$; $\delta_p = 12.34$; $\delta_h = 12.50$; $R_{Sol} = 12.4$ MPa^{1/2}] and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. **(b)** Centre, radius and outliers of the gelation sphere from the NO method and the AO method.

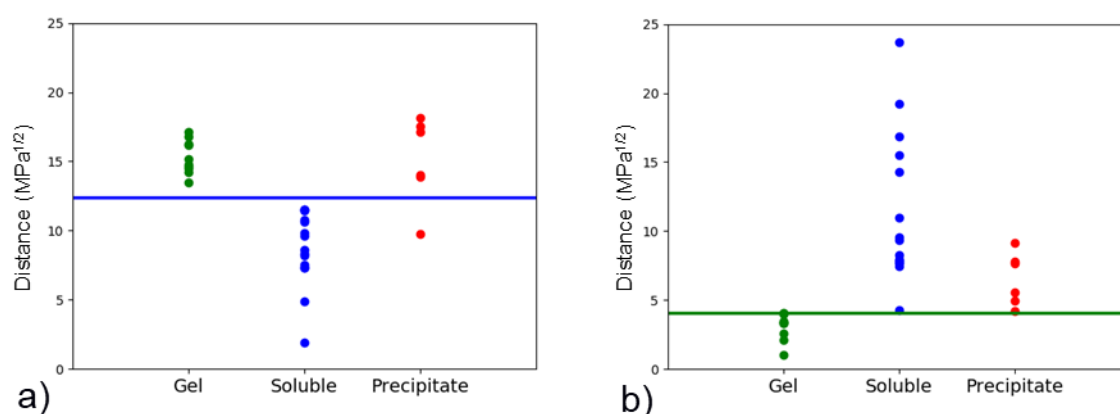


Figure S17. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG **a1** (AO method). The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble.

3. AO method applied to other studies

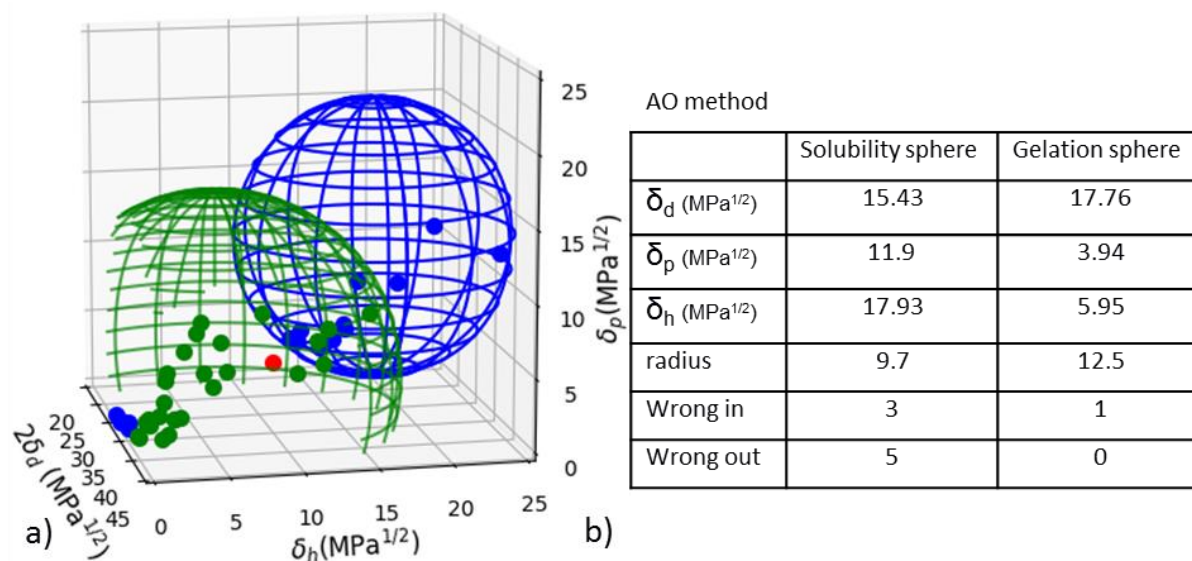


Figure S18. (a) Solubility data for methyl 4,6-O-(p-chlorobenzylidene)- α -D-glucopyranoside gelator reported by Rongxiu Feng et al¹⁵ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. **(b)** Centre, radius and outliers of the solubility and gelation spheres determined by the AO method.

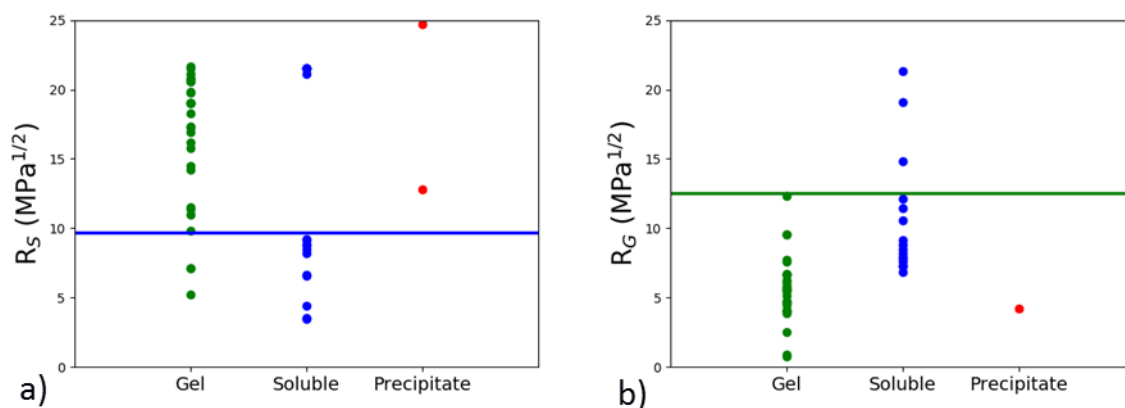


Figure S19. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG presented in Figure S18. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

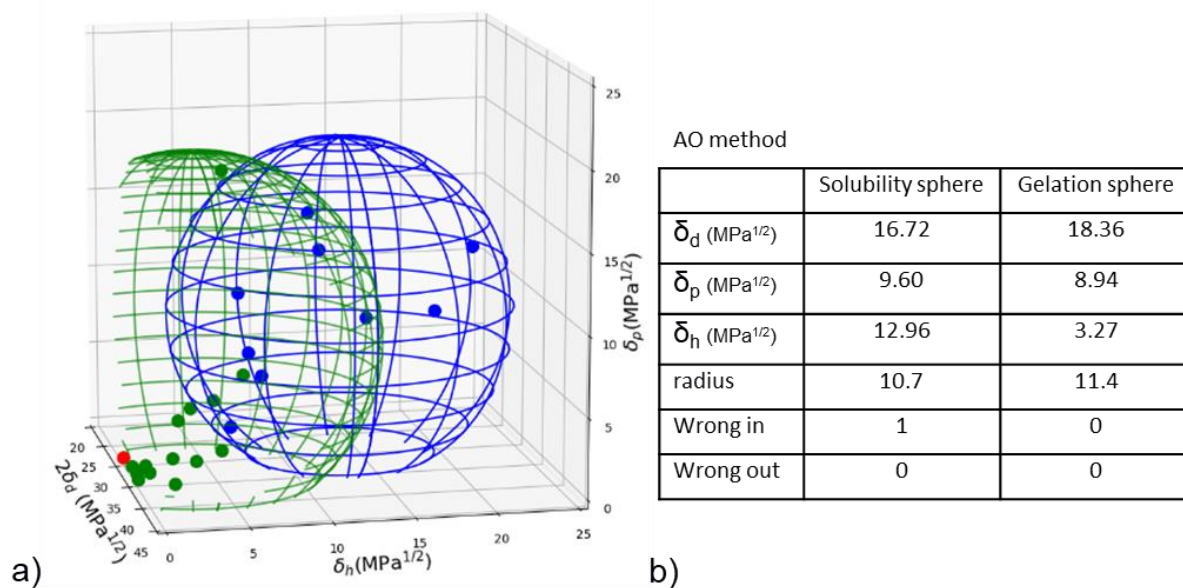


Figure S20. (a) Solubility data for two-component acid–amine gelation system using G2-Lys and C6 and reported by David K. Smith et al¹⁶ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. **(b)** Centre, radius and outliers of the solubility and gelation spheres determined by the AO method. The reliability of the fit is compromised by the limited number of liquids tested (notably liquids with high δ_h values).

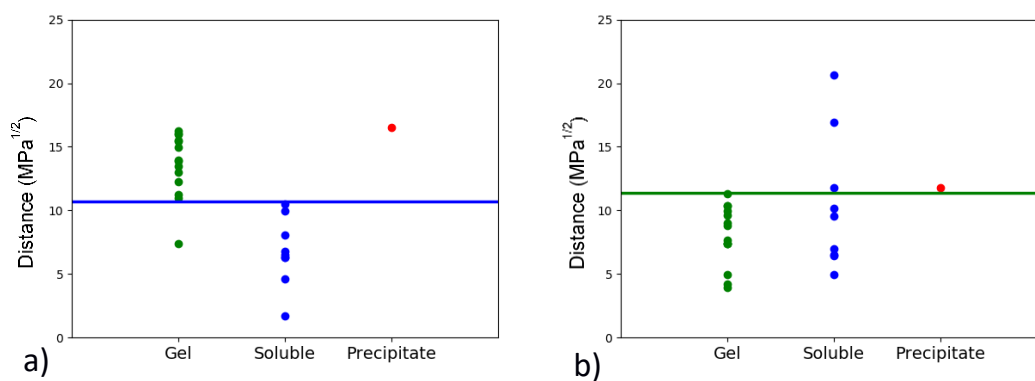


Figure S21. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG presented in Figure S20. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

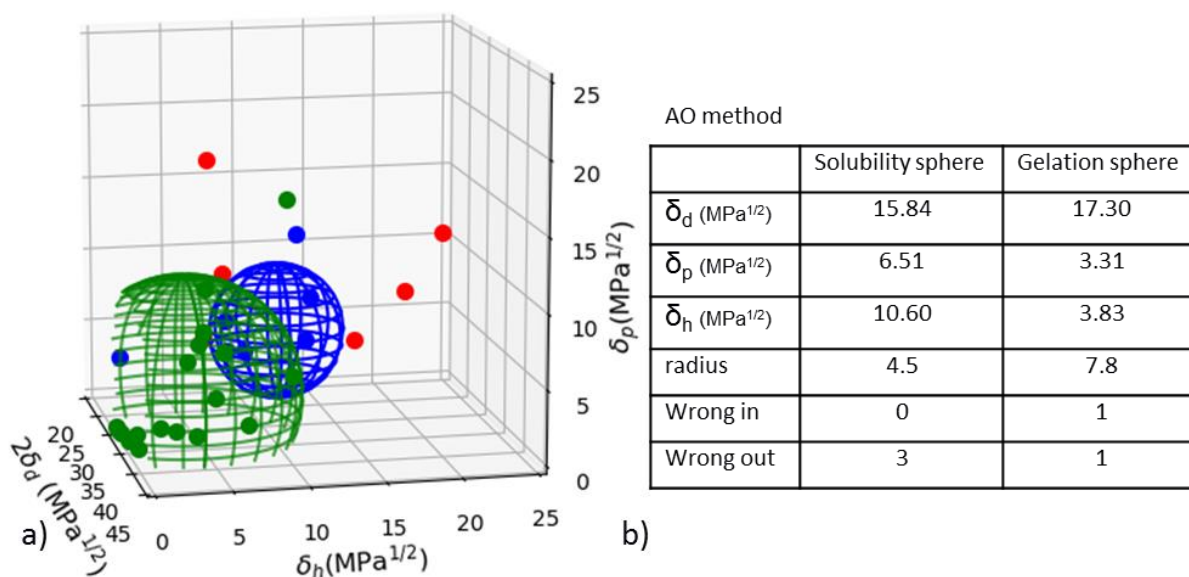


Figure S22. (a) Solubility data for 2,3-dihydroxycholestane steroids gelator reported by Pablo H. Di Chenna et al¹⁷ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. (b) Centre, radius and outliers of the solubility and gelation spheres determined by the AO method.

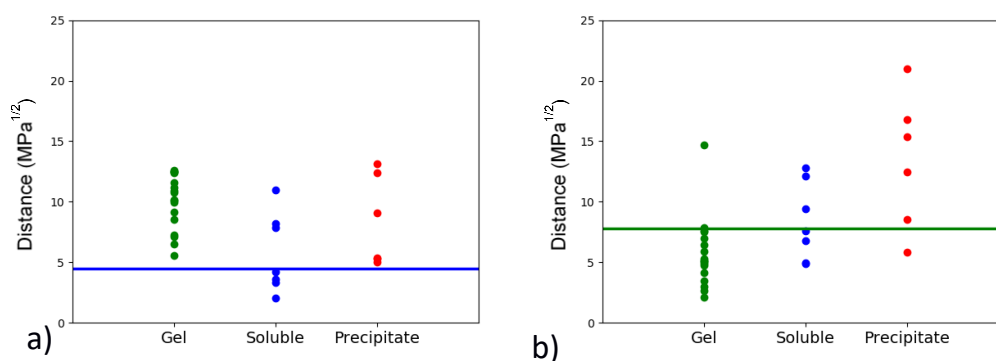


Figure S23. Distances in Hansen space to the centre of the solubility sphere (a) or to the centre of the gelation spheres (b) for LMWG presented in Figure S22. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

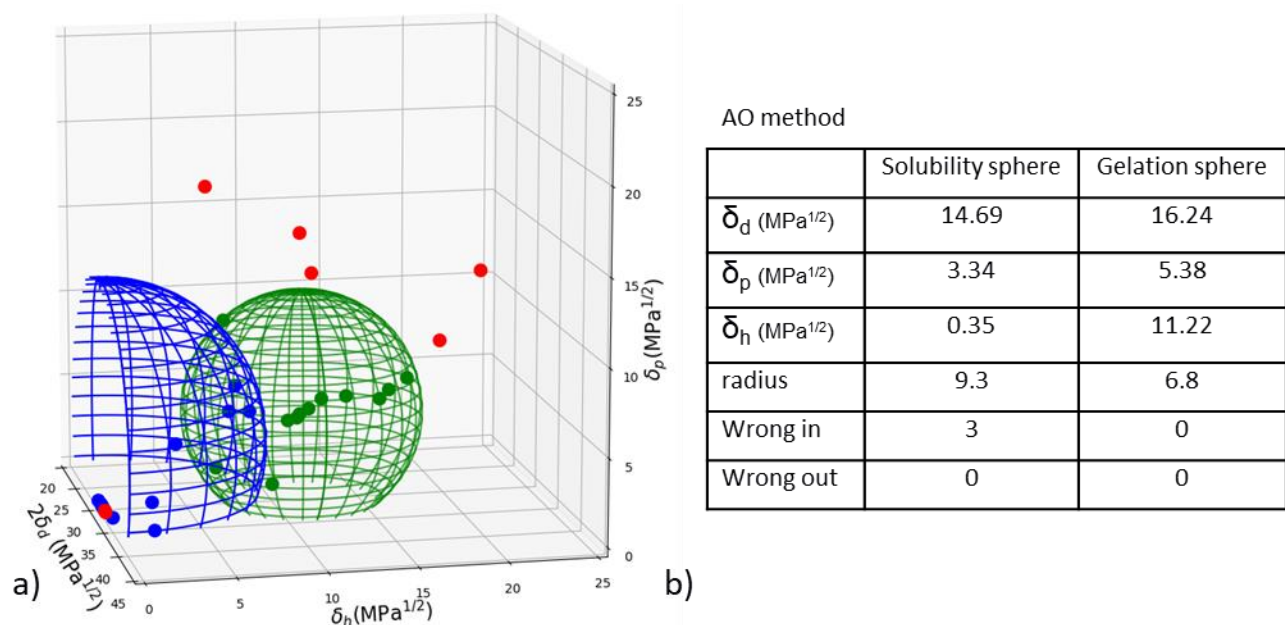


Figure S24. (a) Solubility data for poly(aryl ether)dendron gelator **2a12** reported by Kazuaki Ito et al¹⁸ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. **(b)** Centre, radius and outliers of the solubility and gelation spheres determined by the AO method.

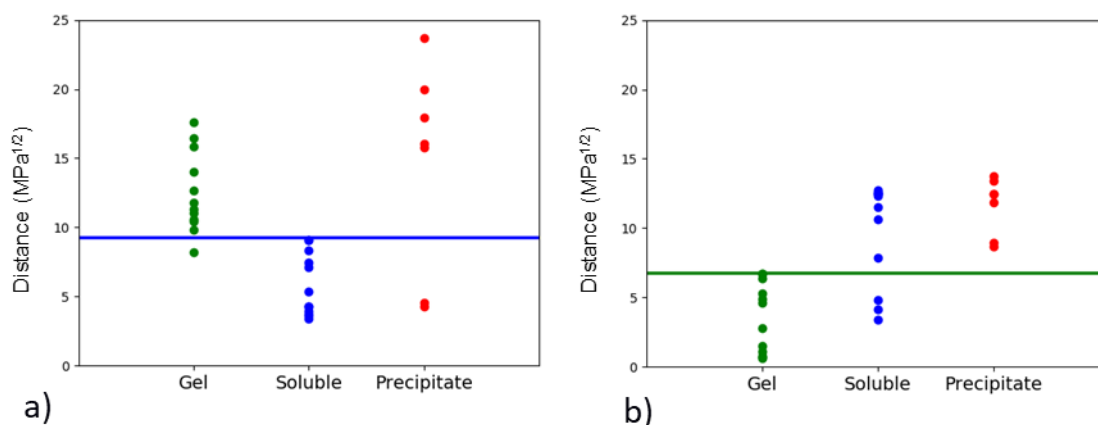


Figure S25. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG presented in Figure S24. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

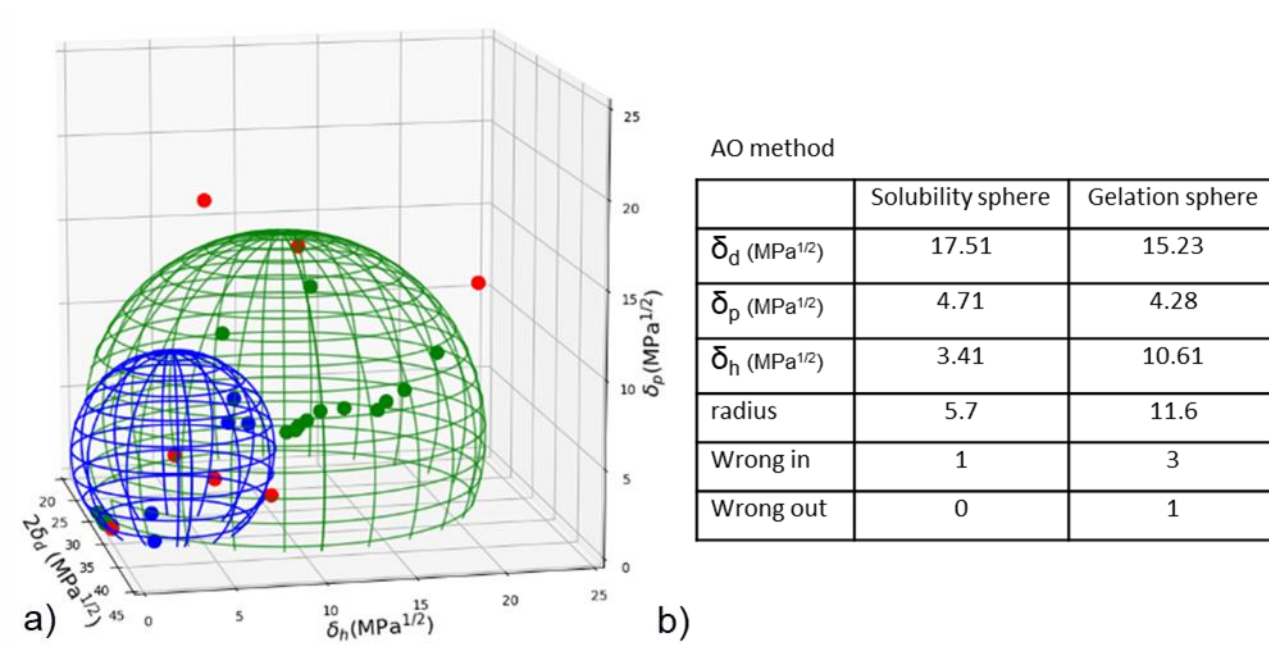


Figure S26. (a) Solubility data for poly(aryl ether)dendron gelator **2b12** reported by Kazuaki Ito et al¹⁸ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. **(b)** Centre, radius and outliers of the solubility and gelation spheres determined by the AO method. The reliability of the fit is compromised by the limited number of liquids tested.

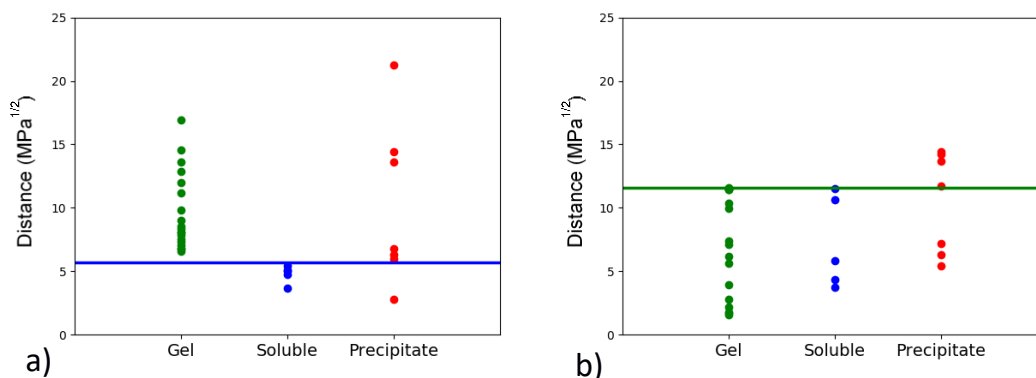


Figure S27. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG presented in Figure S26. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

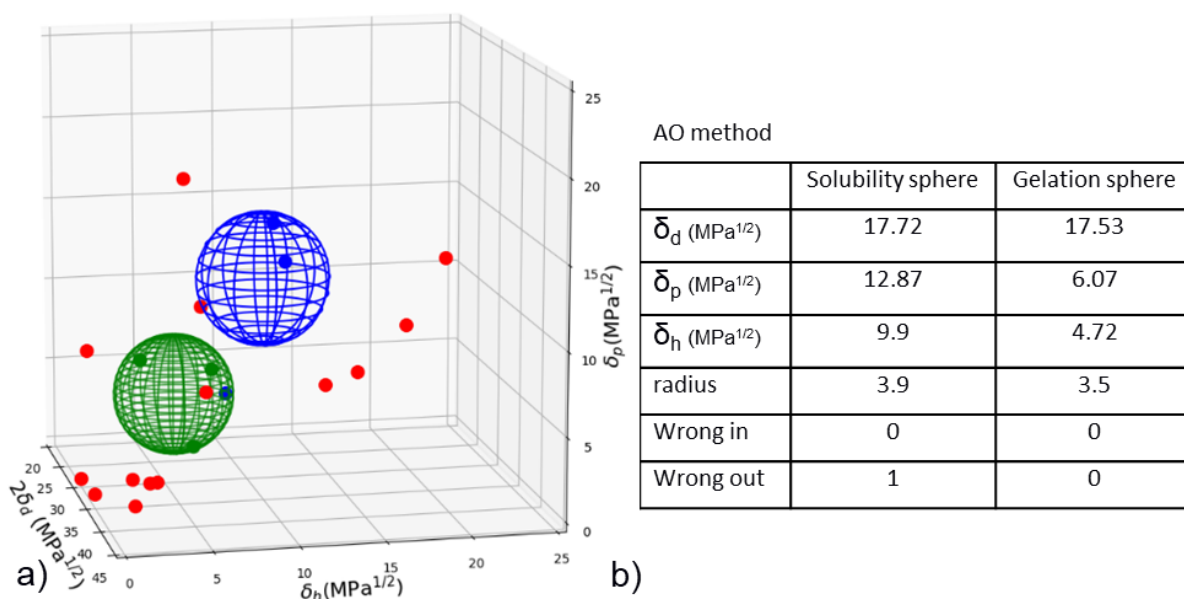


Figure S28. (a) Solubility data for a adenine–thymine(AT) pyrimido[4,5-d]pyrimidine pyranosyl arabinonucleoside gelation system reported by Yang He et al¹⁹ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. (b) Centre, radius and outliers of the solubility and gelation spheres determined by the AO method. The reliability of the fit is compromised by the limited number of liquids tested.

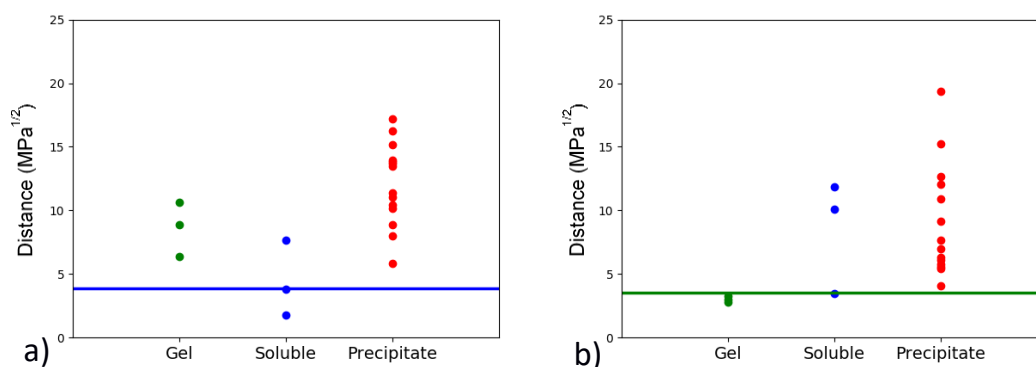


Figure S29. Distances in Hansen space to the centre of the solubility sphere (a) or to the centre of the gelation sphere (b) for LMWG presented in Figure S28. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

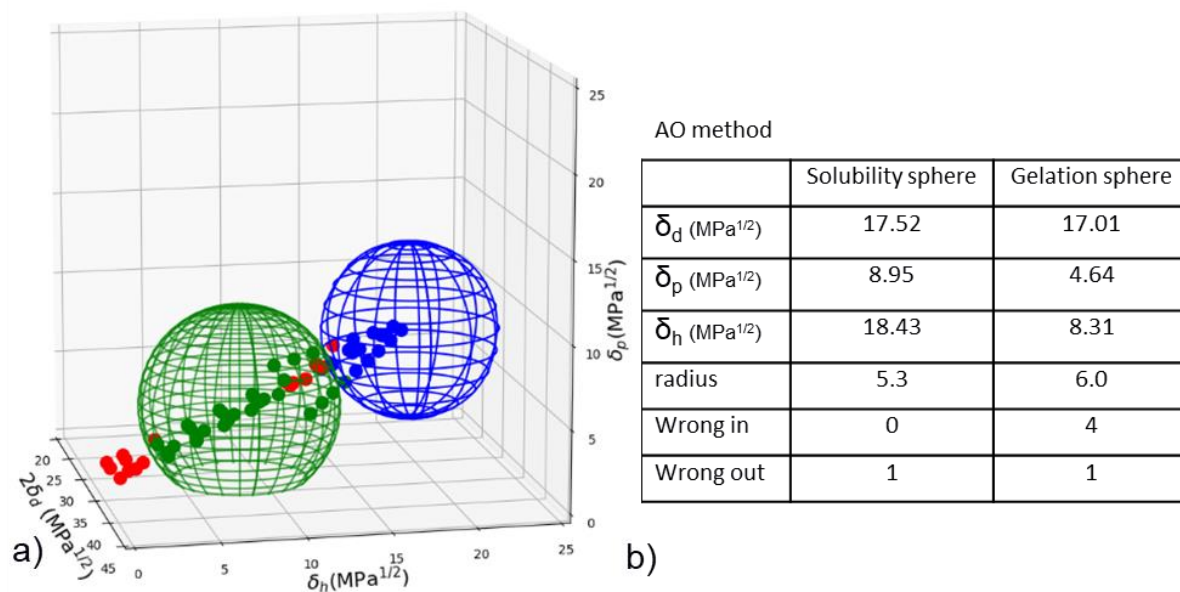


Figure S30. (a) Solubility data for D-sorbitol-based gelation system reported by Jian Song et al²⁰ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. **(b)** Centre, radius and outliers of the solubility and gelation spheres determined by the AO method. The reliability of the fit is compromised by the limited number of liquids tested.

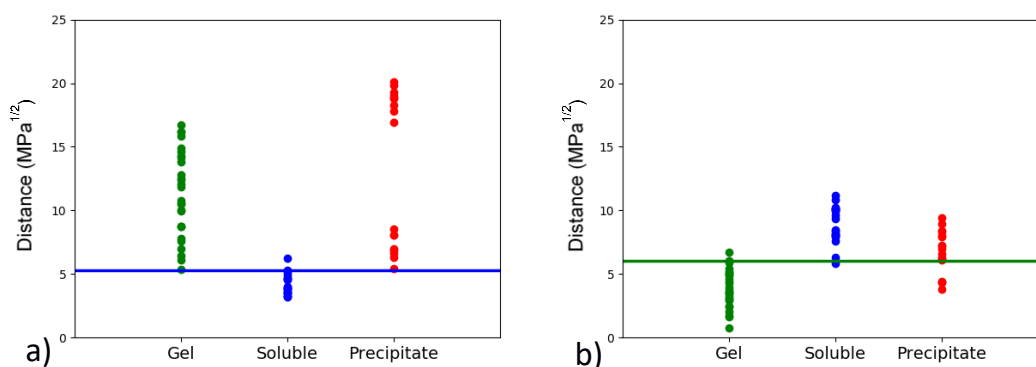


Figure S31. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG presented in Figure S30. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

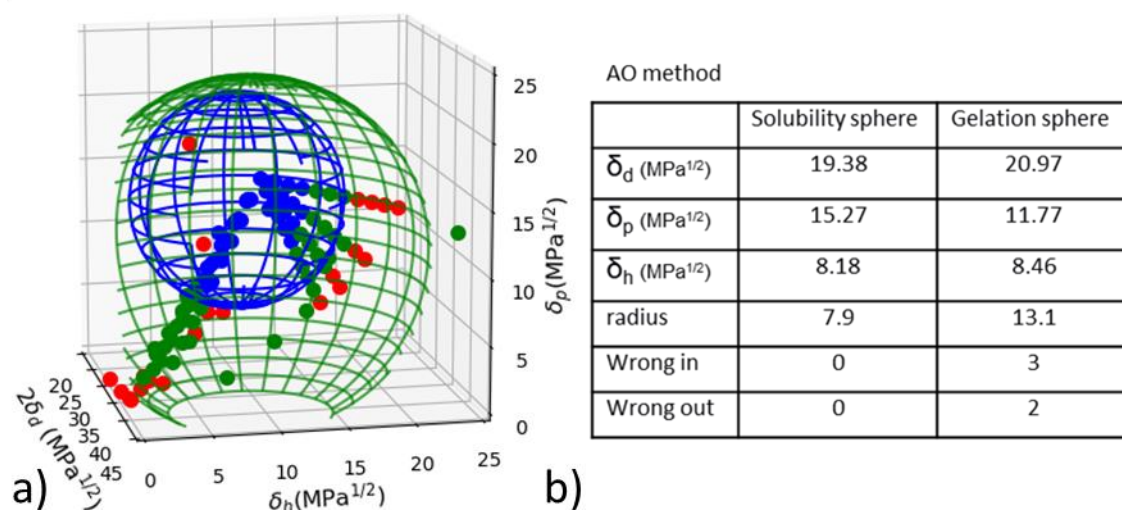


Figure S32. (a) Solubility data for 1,3:2,4-bis(3,4-dimethylbenzylidene)sorbitol gelator reported by Jian Song et al²¹ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. (b) Centre, radius and outliers of the solubility and gelation spheres determined by the AO method. The reliability of the fit is compromised by the limited number of liquids surrounding the solubility sphere.

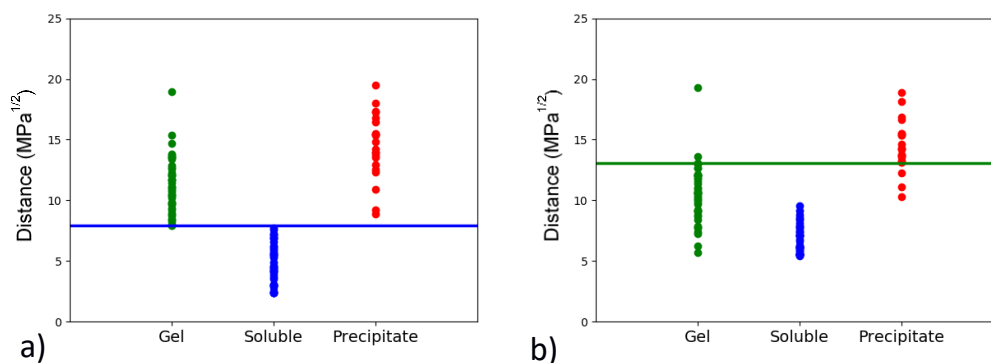


Figure S33. Distances in Hansen space to the centre of the solubility sphere (a) or to the centre of the gelation sphere (b) for LMWG presented in Figure S32. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

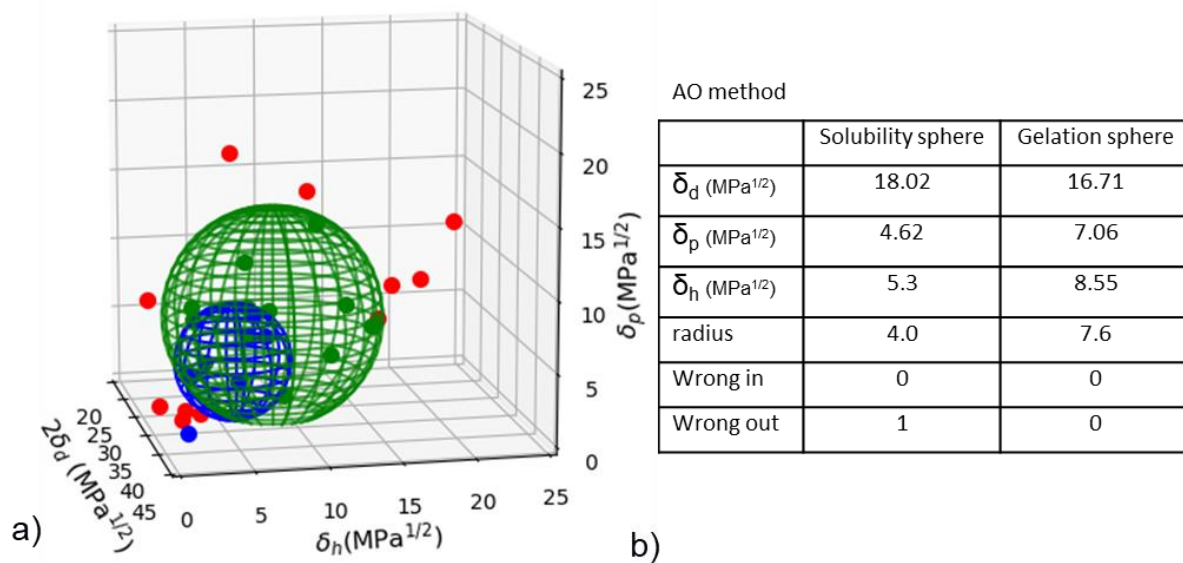


Figure S34. (a) Solubility data for gelator **6a** reported by Hongmei Qu et al²² represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. **(b)** Centre, radius and outliers of the solubility and gelation spheres determined by the AO method.

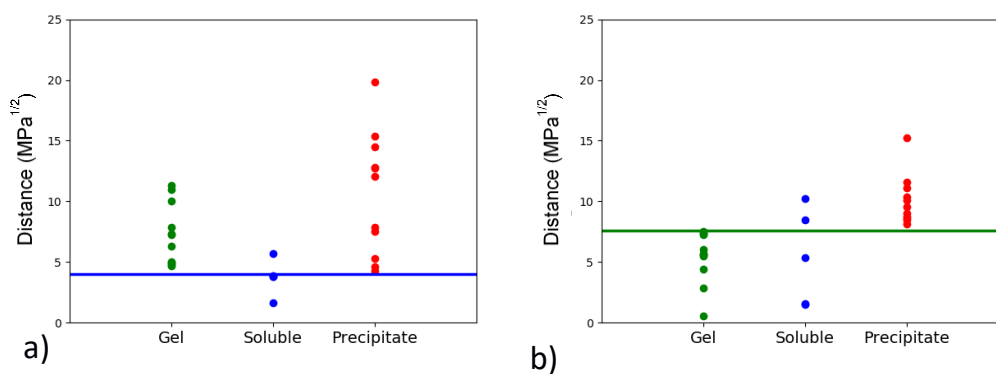


Figure S35. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG presented in Figure S34. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

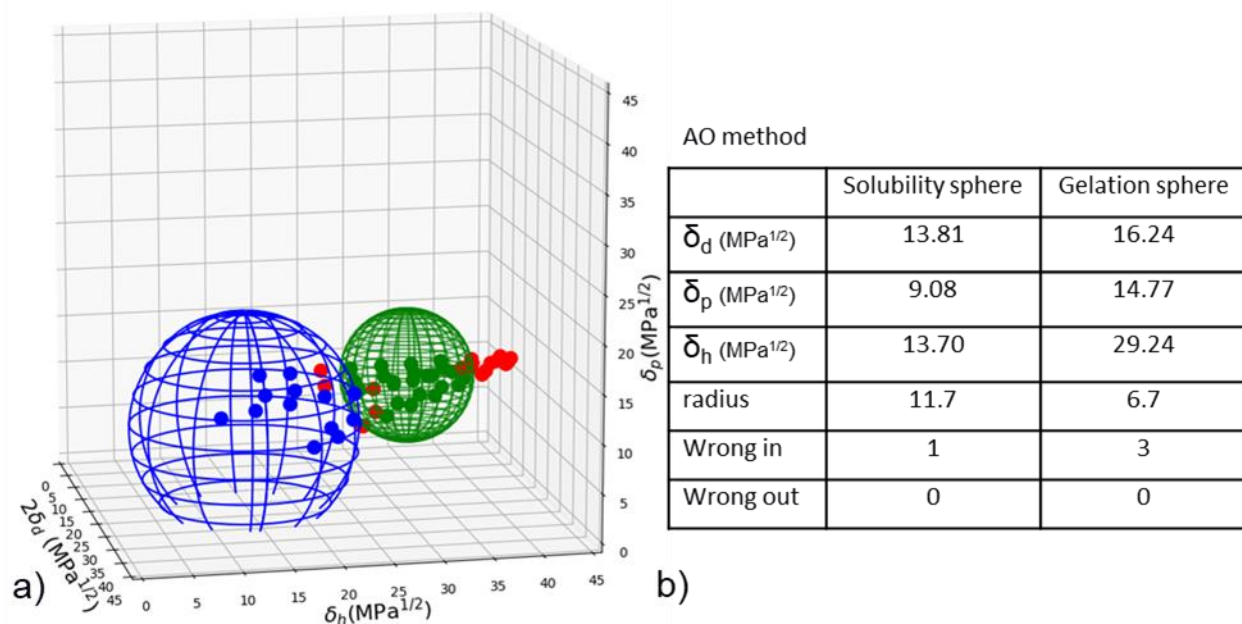


Figure S36. (a) Solubility data for hydrazine derived gelation system reported by Lijun Guo et al²³ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. **(b)** Centre, radius and outliers of the solubility and gelation spheres determined by the AO method. The reliability of the fit is compromised by the limited number of liquids surrounding the solubility sphere.

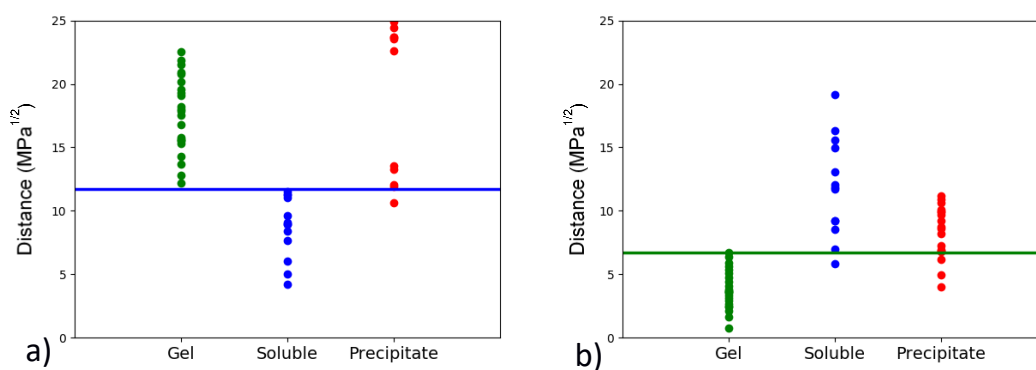


Figure S37. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation spheres **(b)** for LMWG presented in Figure S36. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

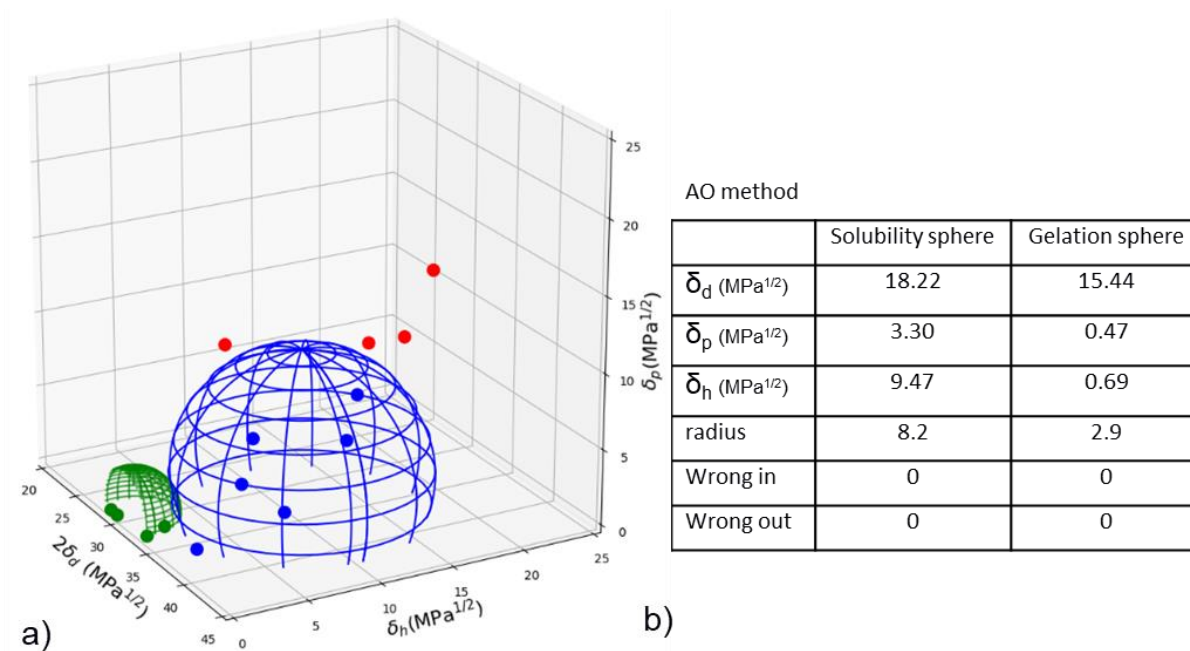


Figure S38. (a) Solubility data for cholesterol-based gelation system reported by Xiaoli Zhen et al²⁴ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. **(b)** Centre, radius and outliers of the solubility and gelation spheres determined by the AO method. The reliability of the fit is compromised by the limited number of liquids tested.

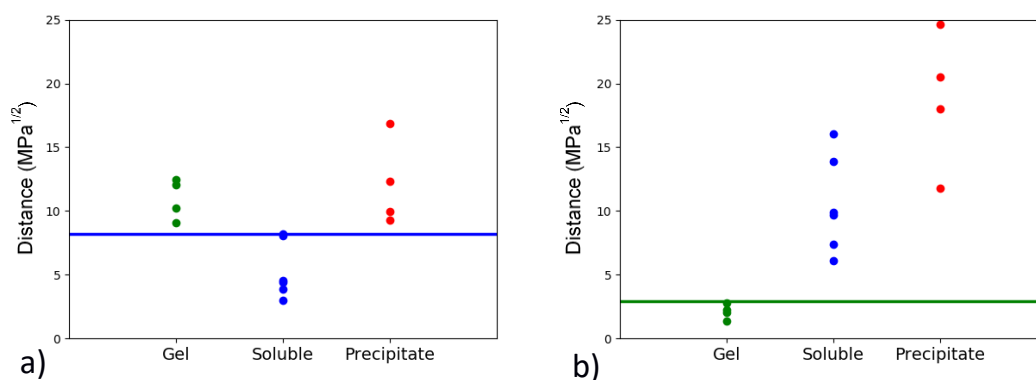


Figure S39. Distances in Hansen space to the centre of the solubility sphere **(a)** or to the centre of the gelation sphere **(b)** for LMWG presented at Figure S38. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

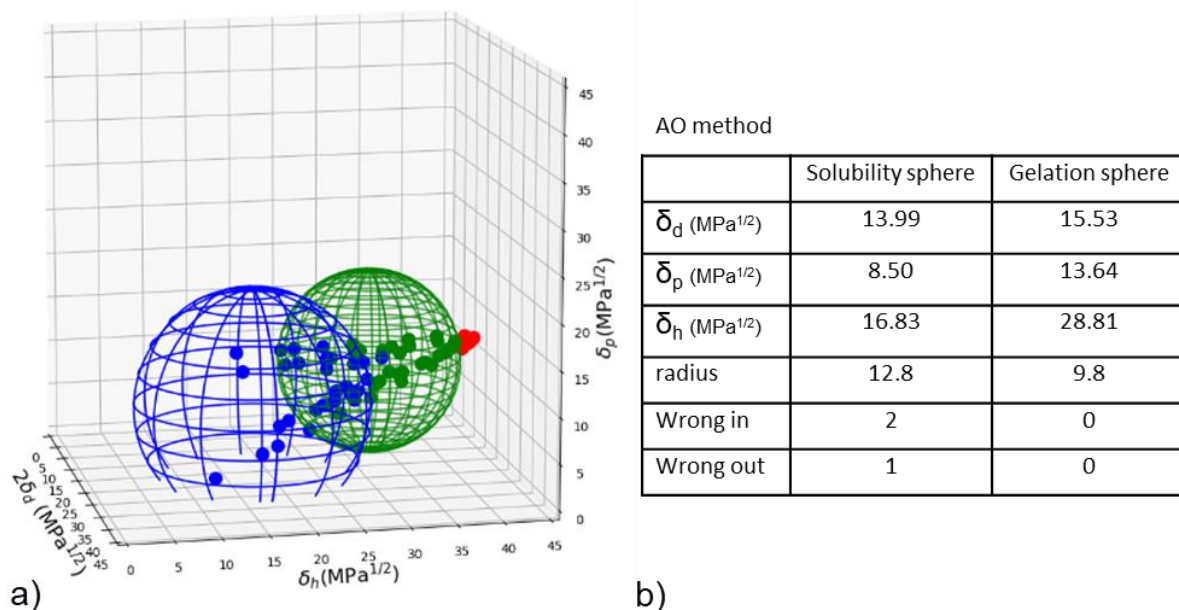


Figure S40. (a) Solubility data for bis-dipeptide based gelation system reported by Yong Yang et al²⁵ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. (b) Centre, radius and outliers of the solubility and gelation spheres determined by the AO method. The reliability of the fit is compromised by the limited number of liquids surrounding the solubility sphere.

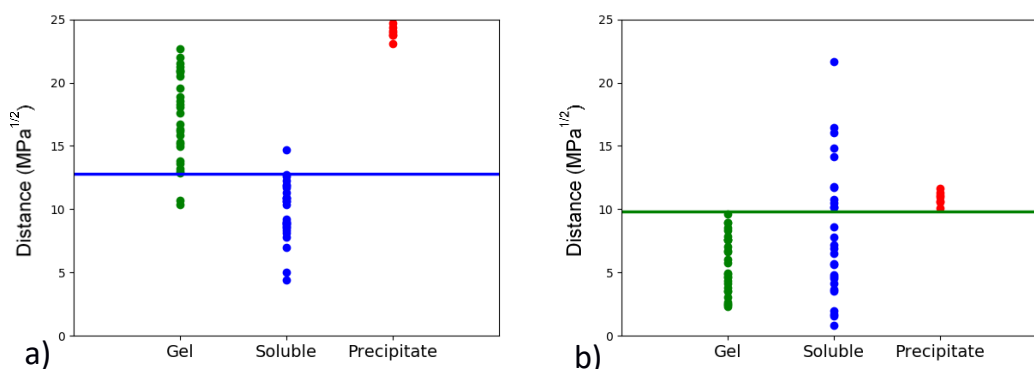


Figure S41. Distances in Hansen space to the centre of the solubility sphere (a) or to the centre of the gelation sphere (b) for LMWG presented in Figure S40. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

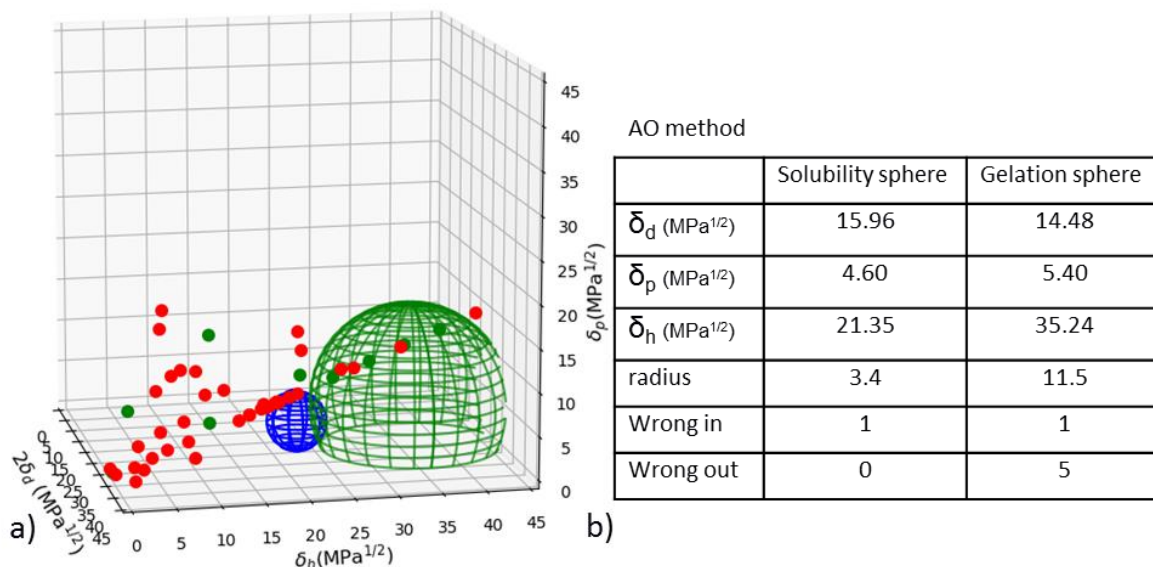


Figure S42. (a) Solubility data for 1,3:2,5:4,6-tris(3,4-dichlorobenzylidene)-*D*-mannitol gelator reported by Bao Zhang et al²⁶ represented in Hansen space. Liquids are represented by full circles and calculated domains are represented by meshed spheres. Green: gel; Red: precipitate. Blue: soluble. The solubility sphere was calculated using the HSPiP³⁻⁵ software and the gelation sphere was calculated with the AO method using the HSPiP³⁻⁵. (b) Centre, radius and outliers of the solubility and gelation spheres determined by the AO method. The reliability of the fit is compromised by the limited number of liquids tested.

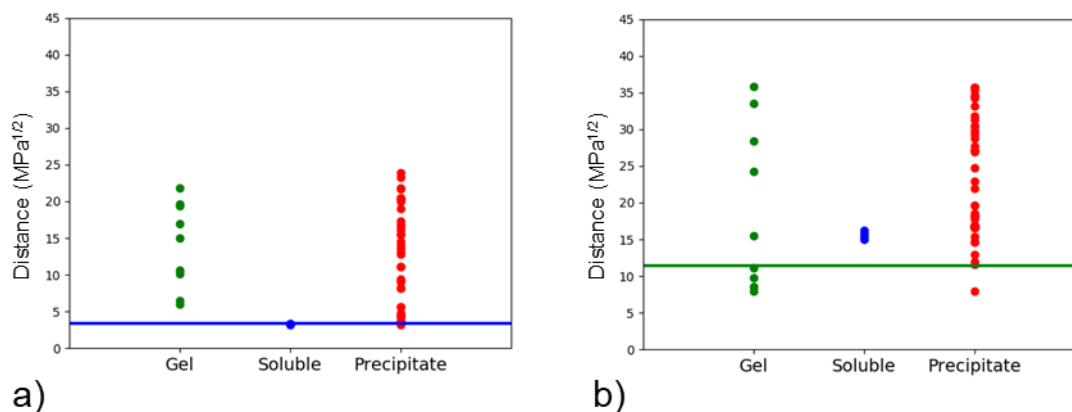
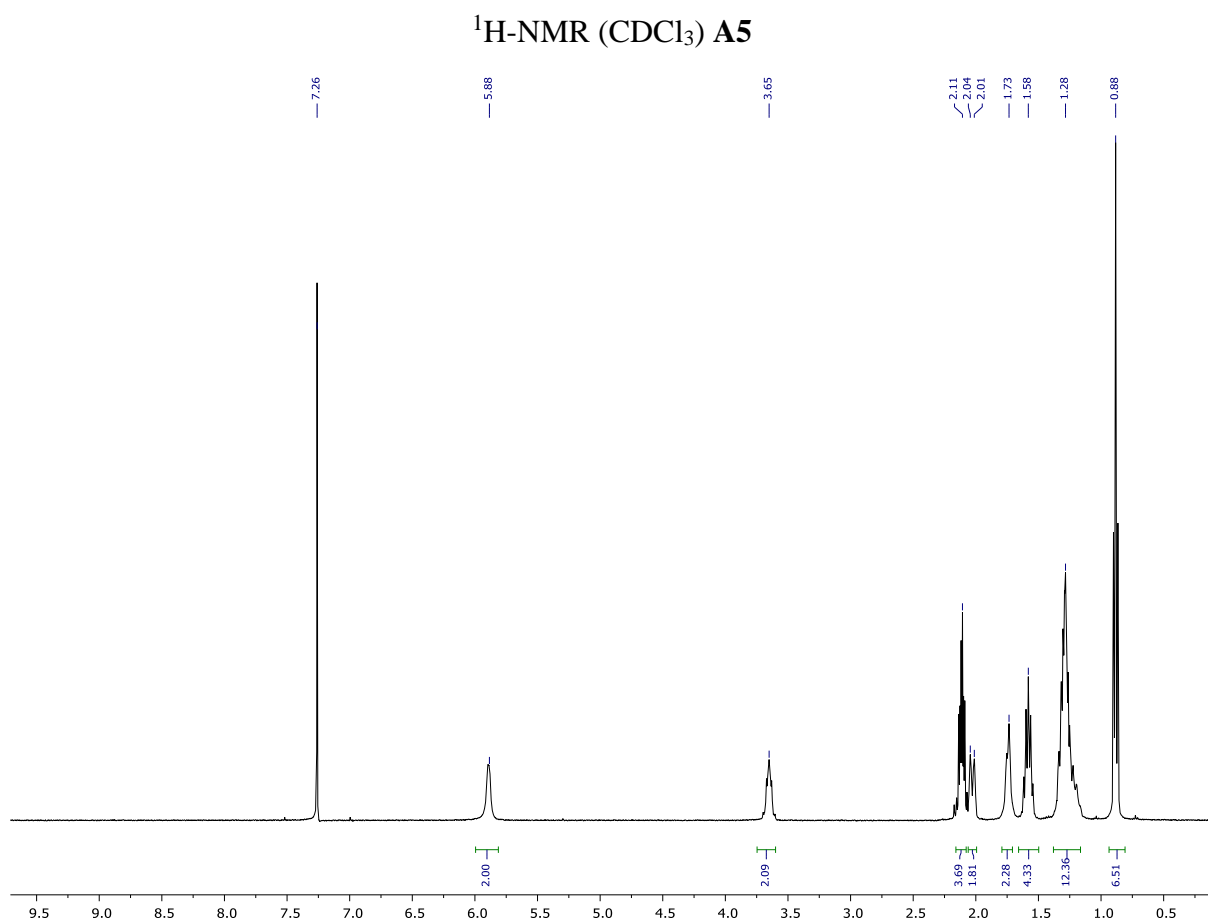


Figure S43. Distances in Hansen space to the centre of the solubility sphere (a) or to the centre of the gelation sphere (b) for LMWG presented at Figure S42. The lines represent the radius of the spheres. Green: gel; Red: precipitate. Blue: soluble

4. NMR spectrum for LMWG A5



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