Electronic Supplementary Material (ESI) for Chemical Communications

Supporting information

Organogel formation rationalized by Hansen solubility parameters

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Procedure for the determination of the centre of the solubility sphere:
In the Excel worksheet provided, the coordinates of the centre (δ_d , δ_p , δ_h) and the radius (R_{sol}) of a sphere were optimized to include as many S points as possible and to exclude as many I and G points as possible.

Procedure for the determination of the centre of the gel sphere:
In the same Excel worksheet, the coordinates of the centre (δ_d , δ_p , δ_h) and the radius (R_{sol}) of a sphere were optimized to include as many G points as possible and to exclude as many I and S points as possible.

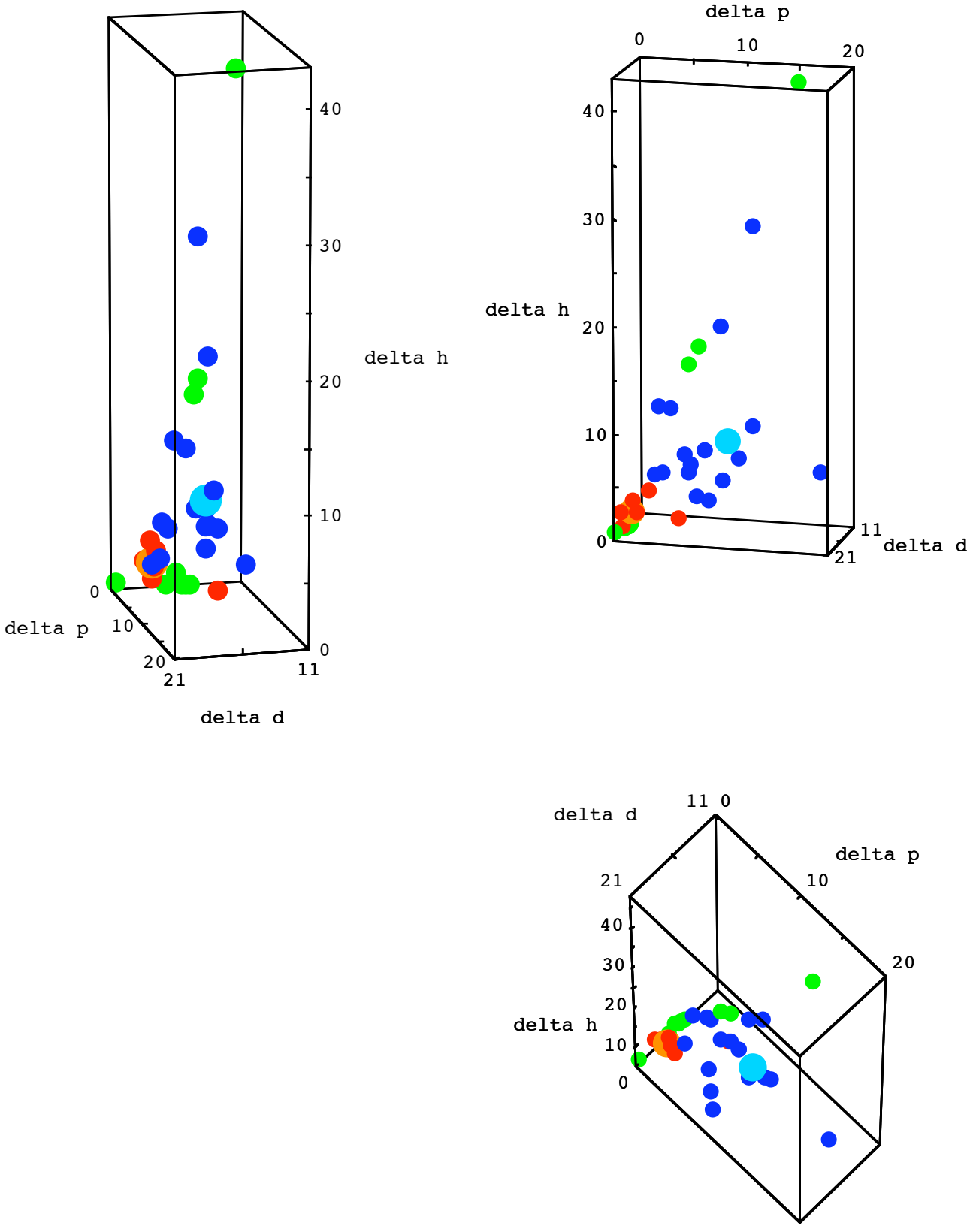

Figure S1. Solubility data for LMWG **1** (30g/L) represented in Hansen space (Units: $MPa^{0.5}$) (data taken from reference 1). Blue: soluble; red: gel; green: insoluble. Cyan: centre of the solubility sphere; orange: centre of the gelation sphere.

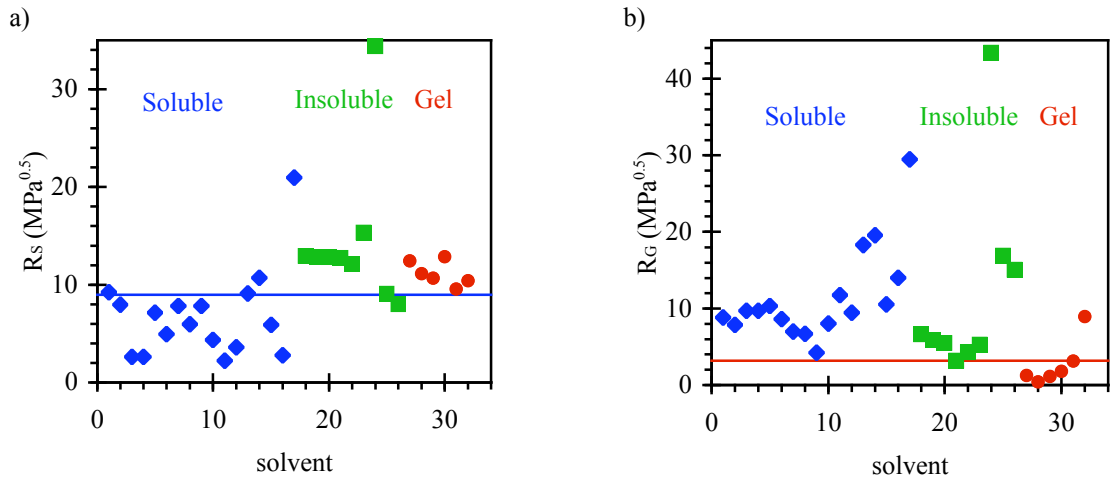

Figure S2. Distances in Hansen space to the centre of the solubility sphere [δ_d = 16.0; δ_p = 9.4; δ_h = 8.7; R_{Sol} = 9.0 MPa$^{0.5}$] (a) or to the centre of the gelation sphere [δ_d = 18.0; δ_p = 1.0; δ_h = 2.0; R_{Gel} = 3.2 MPa$^{0.5}$] (b) for LMWG **1**. The line represents the radius of the sphere. Blue: soluble; red: gel; green: insoluble.

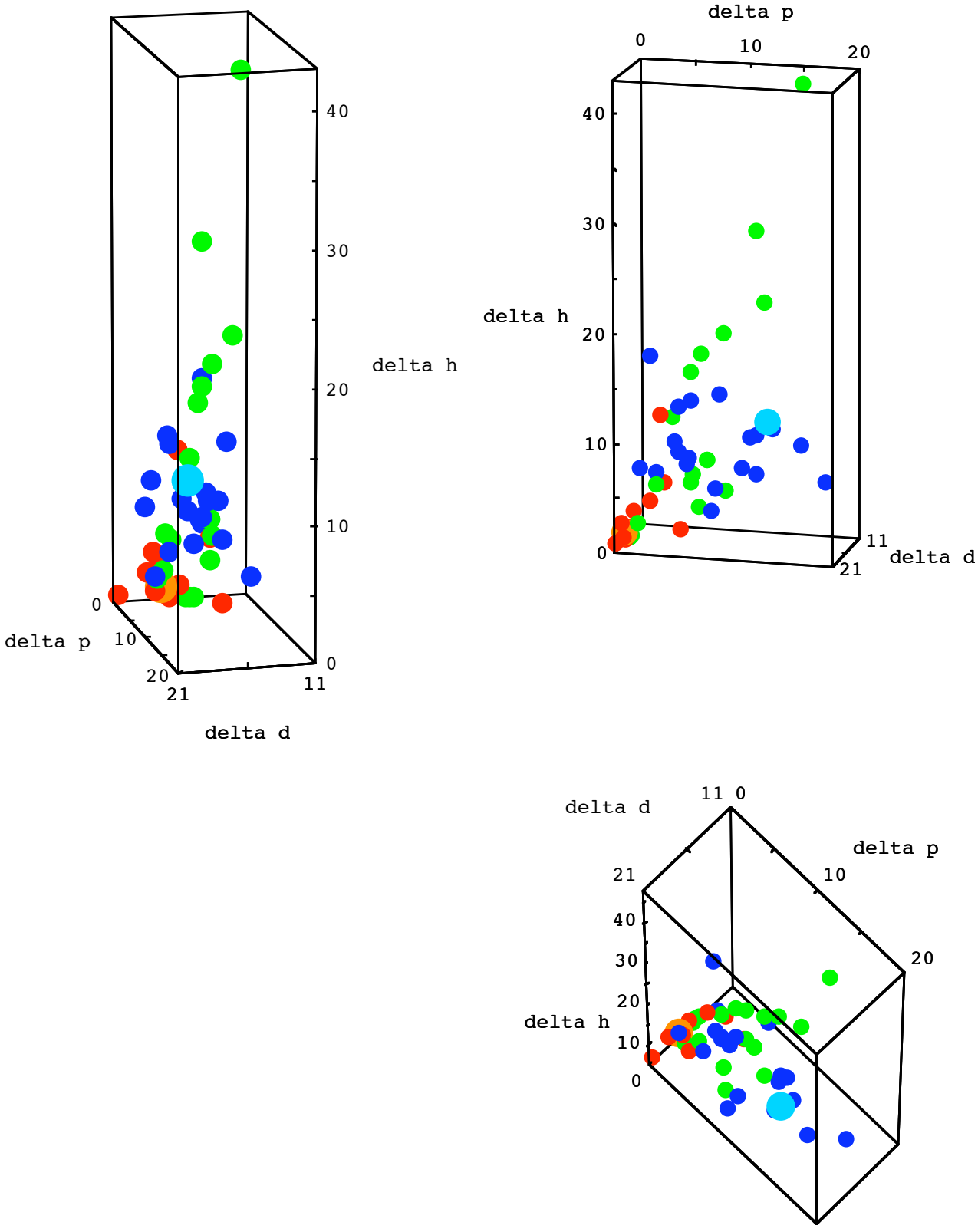

Figure S3. Solubility data for LMWG **2** (30g/L, room temperature) represented in Hansen space (Units: $MPa^{0.5}$) (data taken from reference 2). Blue: soluble; red: gel; green: insoluble. Cyan: centre of the solubility sphere; orange: centre of the gelation sphere.

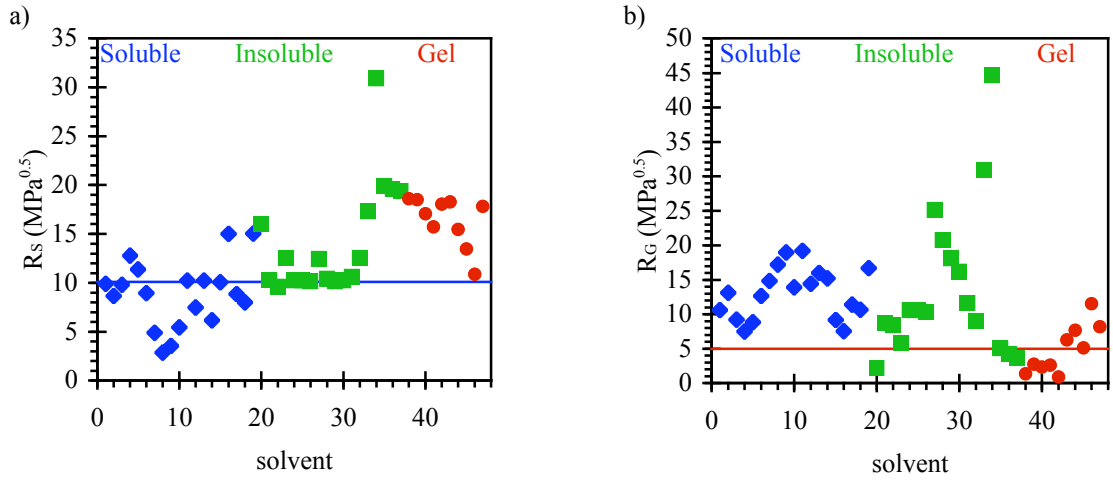

Figure S4. Distances in Hansen space to the centre of the **solubility sphere** [δ_d = 18.7; δ_p = 13.6; δ_h = 12.3; R_{Sol} = 10.1 $MPa^{0.5}$] (a) or to the centre of the **gelation sphere** [δ_d = 17.4; δ_p = 0.0; δ_h = 0.9; R_{Gel} = 5.0 $MPa^{0.5}$] (b) for LMWG **2**. The line represents the radius of the sphere. Blue: soluble; red: gel; green: insoluble.

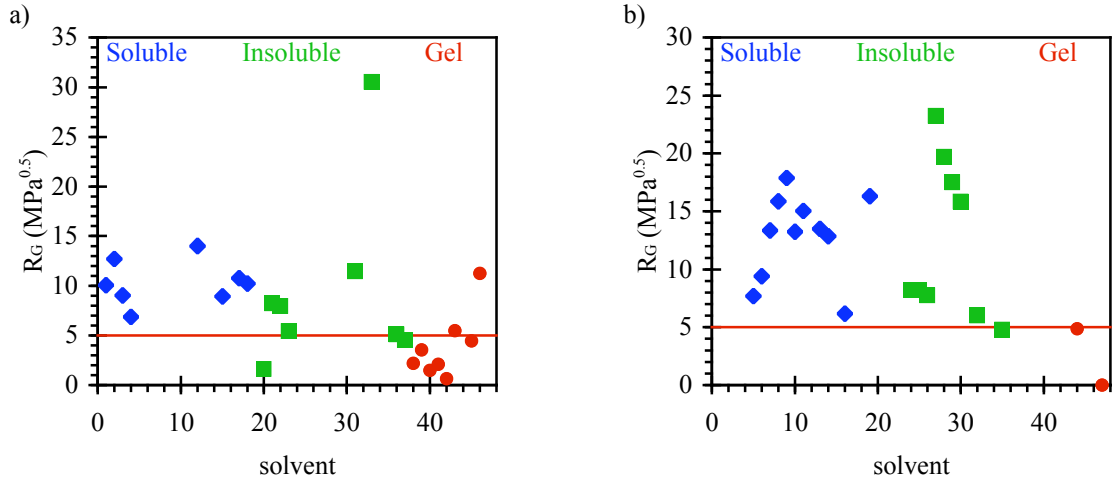

Figure S5. *A better correlation is obtained by considering 2 gelation spheres: the same data as in figure S4b is plotted again. Each solvent is represented only once, either in figure S5a or in figure S5b: only the shortest distance to the gelation sphere centers is considered.* Distances in Hansen space to the centre of the **first gelation sphere** [δ_d = 17.8; δ_p = 0.0; δ_h = 1.2; R_{Gel} = 5.0] (a) or to the centre of the **second gelation sphere** [δ_d = 13.9; δ_p = 4.3; δ_h = 0.6; R_{Gel} = 5.0] (b) for LMWG **2**. The line represents the radius of the sphere. Blue: soluble; red: gel; green: insoluble.

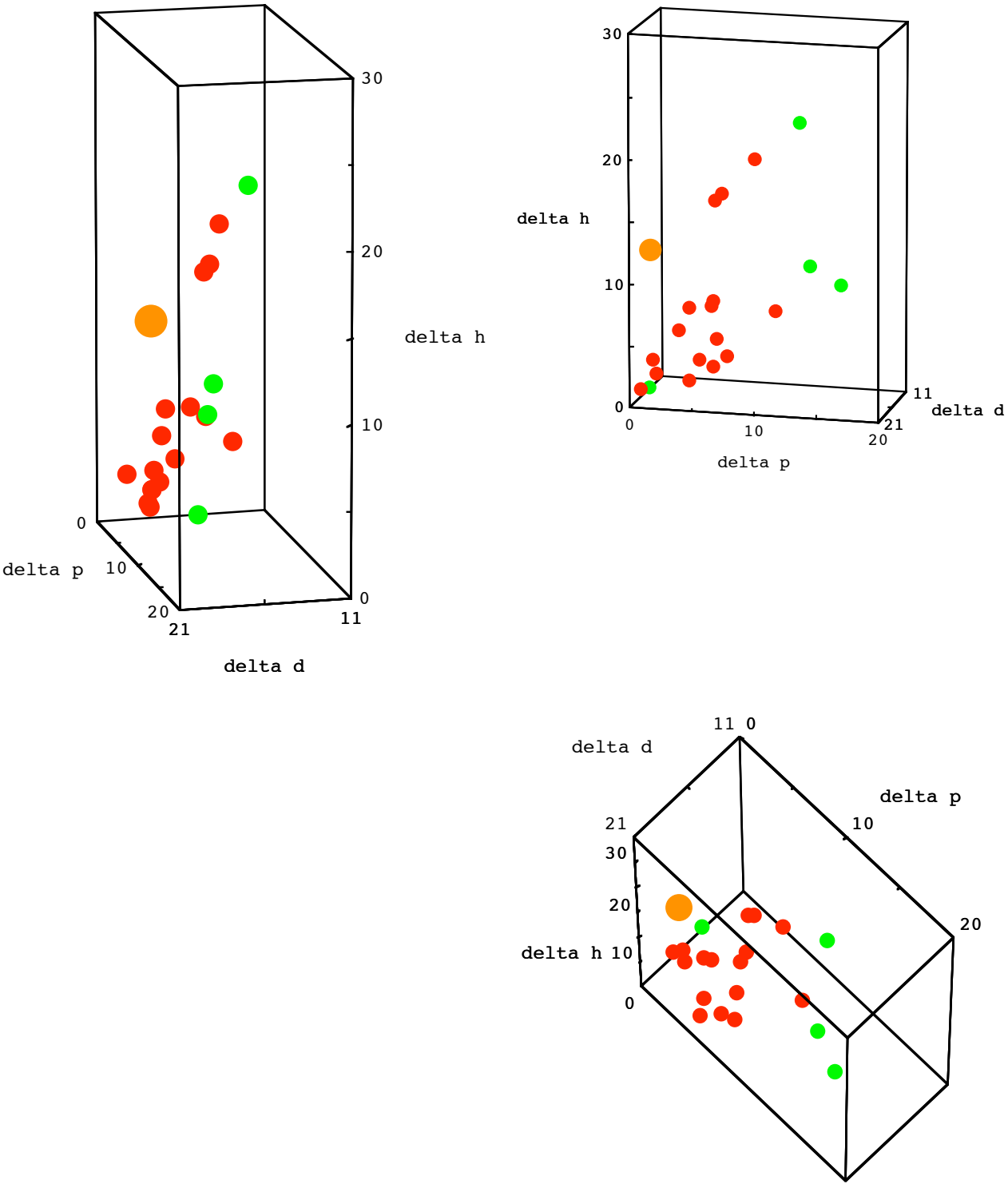

Figure S6. Solubility data for LMWG **3** (< 40mM, room temperature) represented in Hansen space (Units: $MPa^{0.5}$) (data taken from reference 3). Red: gel; green: insoluble. Orange: centre of the gelation sphere. *Good solvents (S) for this system were not reported, but it does not prevent the determination of a gelation sphere.*

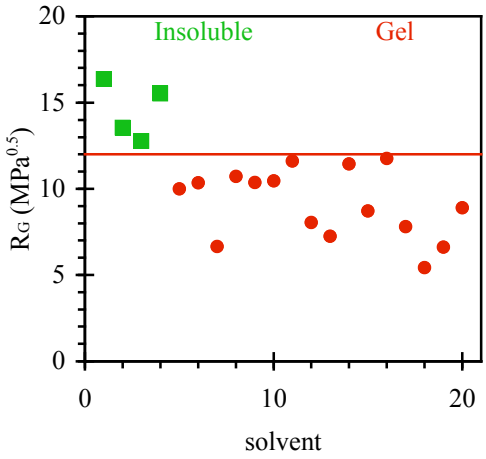

Figure S7. Distances in Hansen space to the centre of the **gelation sphere** [δ_d = 18.0; δ_p = 1.0; δ_h = 12.0; R_{Gel} = 12.0 MPa$^{0.5}$] for LMWG **3**. The line represents the radius of the sphere. Red: gel; green: insoluble.

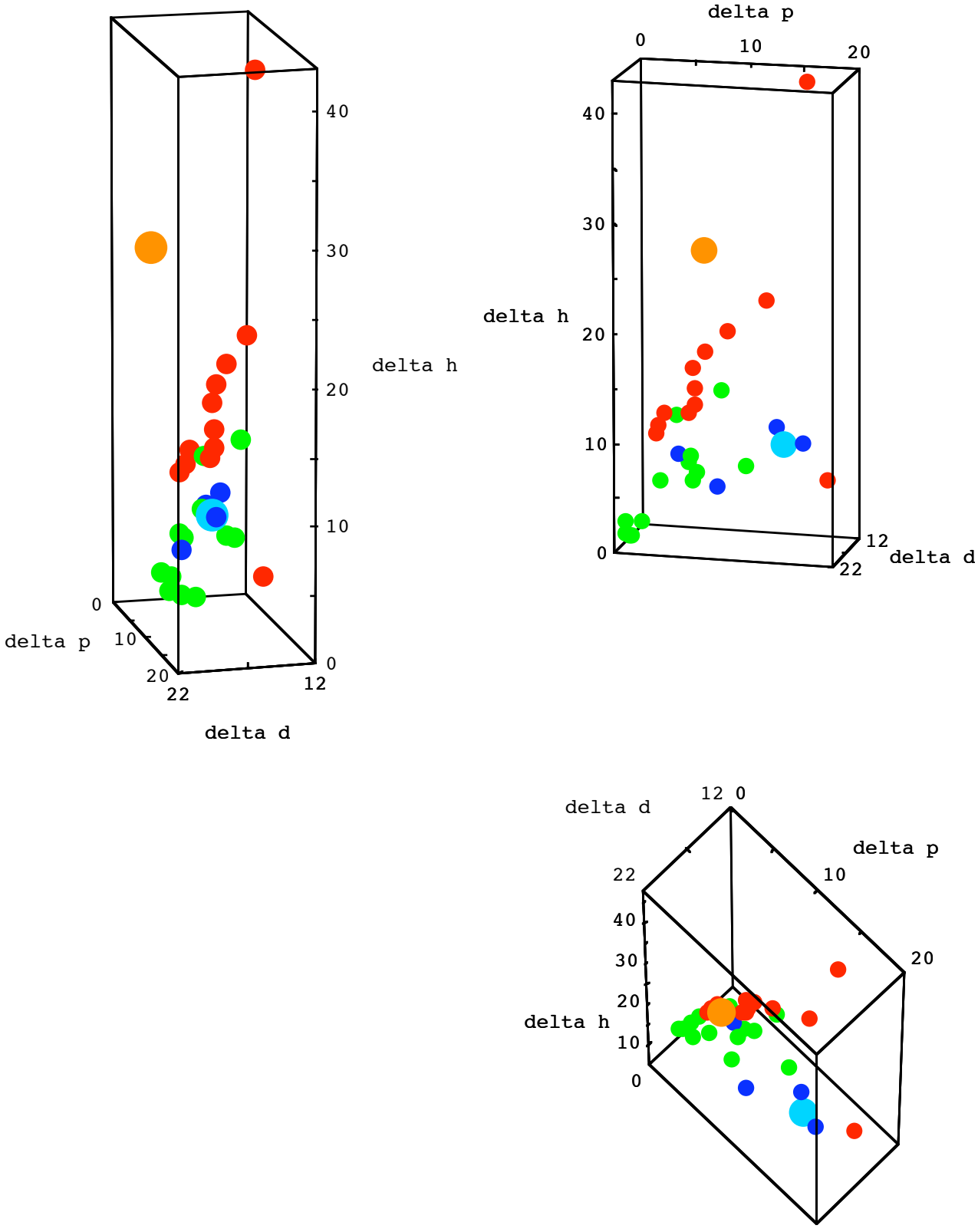

Figure S8. Solubility data for LMWG **4** (25g/L, room temperature) represented in Hansen space (Units: $MPa^{0.5}$) (data taken from reference 4). Blue: soluble; red: gel; green: insoluble. Cyan: centre of the solubility sphere; orange: centre of the gelation sphere.

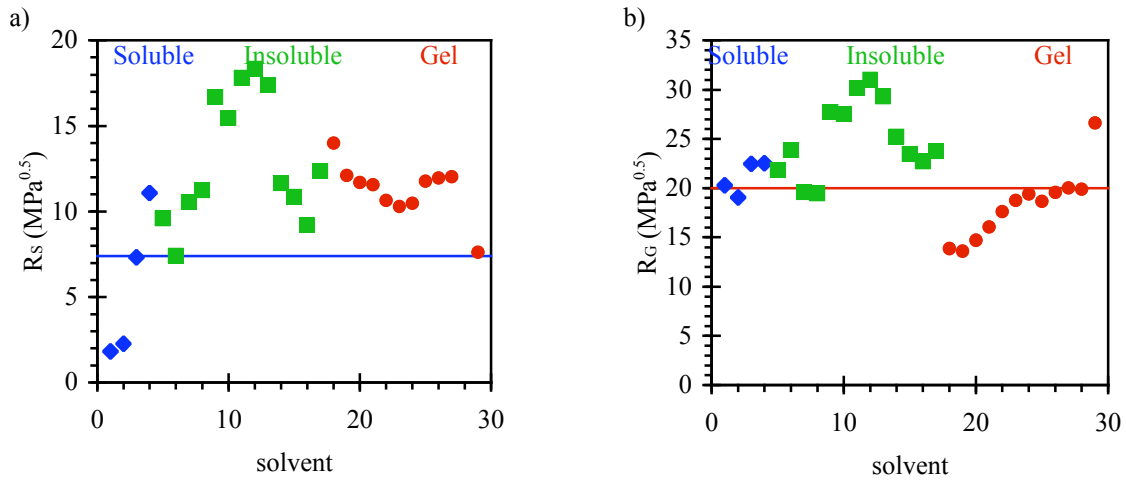

Figure S9. Distances in Hansen space to the centre of the **solubility sphere**[*] [δ_d = 18.2; δ_p = 14.7; δ_h = 9.9; R_{Sol} = 7.4 MPa$^{0.5}$] (a) or to the centre of the **gelation sphere** [δ_d = 21.1; δ_p = 8.2; δ_h = 27.9; R_{Gel} = 20.0 MPa$^{0.5}$] (b) for LMWG **4**. The line represents the radius of the sphere. Blue: soluble; red: gel; green: insoluble.

[*] The location of the solubility sphere is not precise, due to the limited data available (too few good solvents (S)).

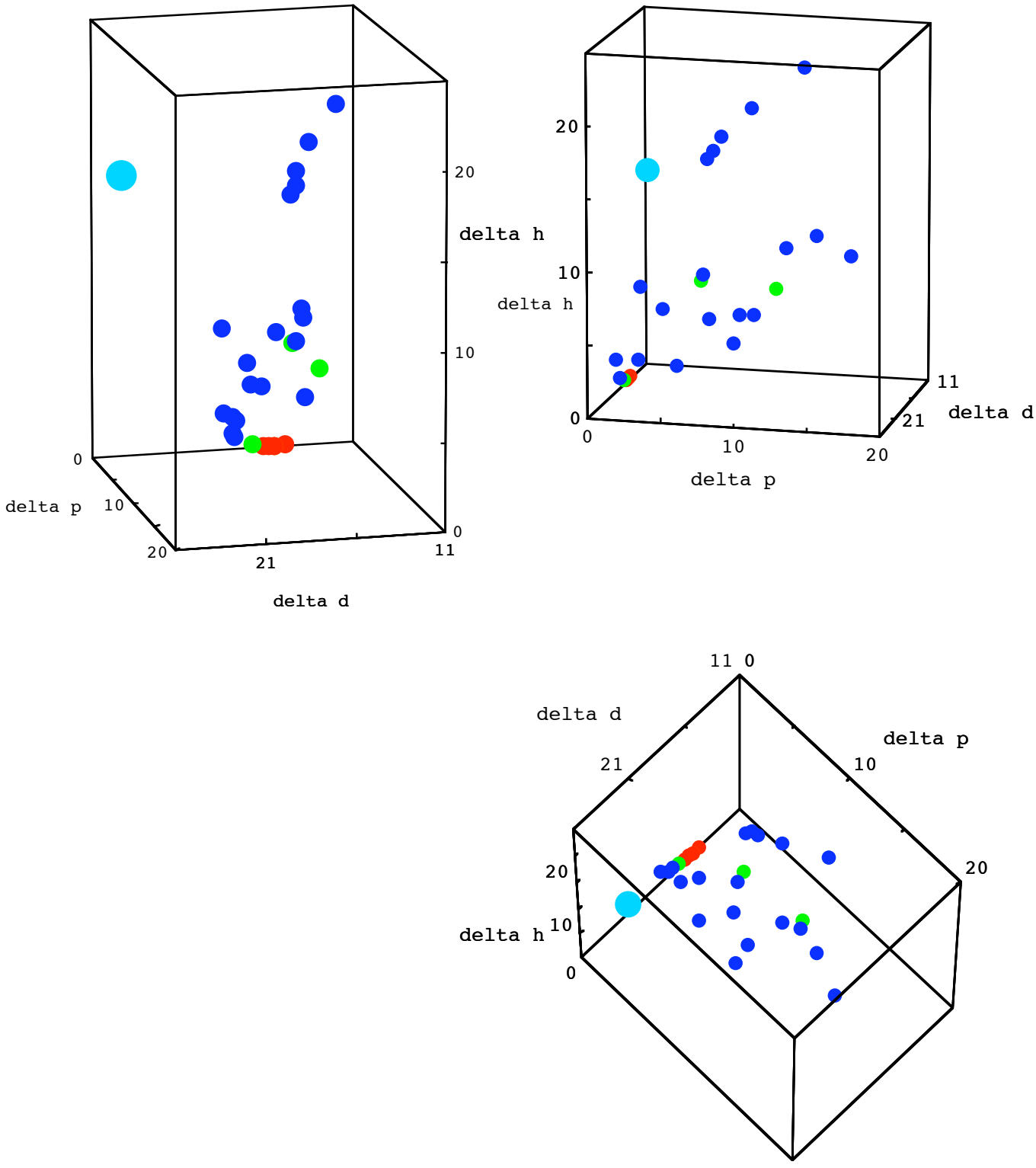

Figure S10. Solubility data for LMWG **5** (< 16g/L, 25°C) represented in Hansen space (Units: $MPa^{0.5}$) (data taken from reference 5). Blue: soluble; red: gel; green: insoluble. Cyan: centre of the solubility sphere.

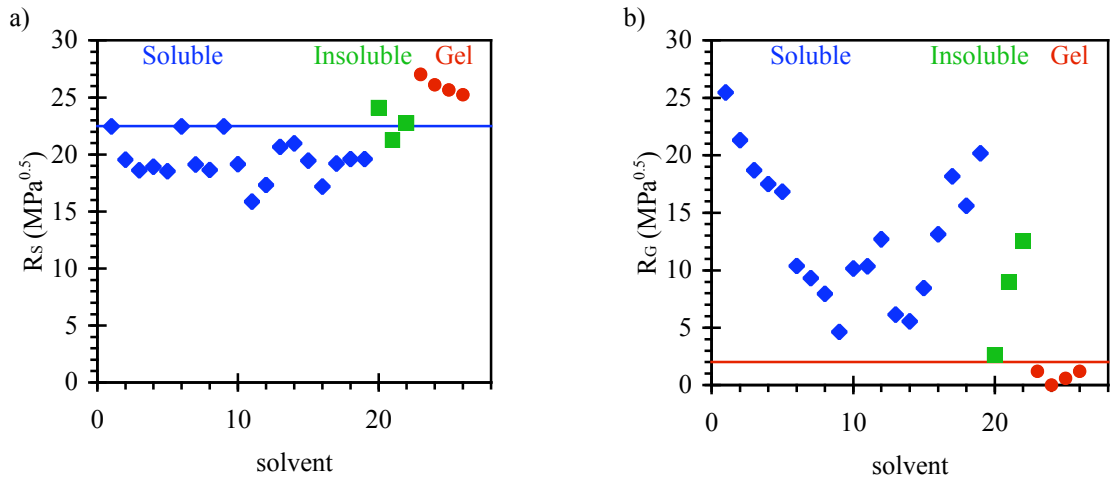

Figure S11. Distances in Hansen space to the centre of the **solubility sphere** [δ_d = 25.2; δ_p = 4.1; δ_h = 17.0; R_{Sol} = 22.5 MPa$^{0.5}$] (a) or to the centre of the **gelation sphere** [δ_d = 15.5; δ_p = 0.0; δ_h = 0.0; R_{Gel} = 2.0 MPa$^{0.5}$] (b) for LMWG **5**. The line represents the radius of the sphere. Blue: soluble; red: gel; green: insoluble.

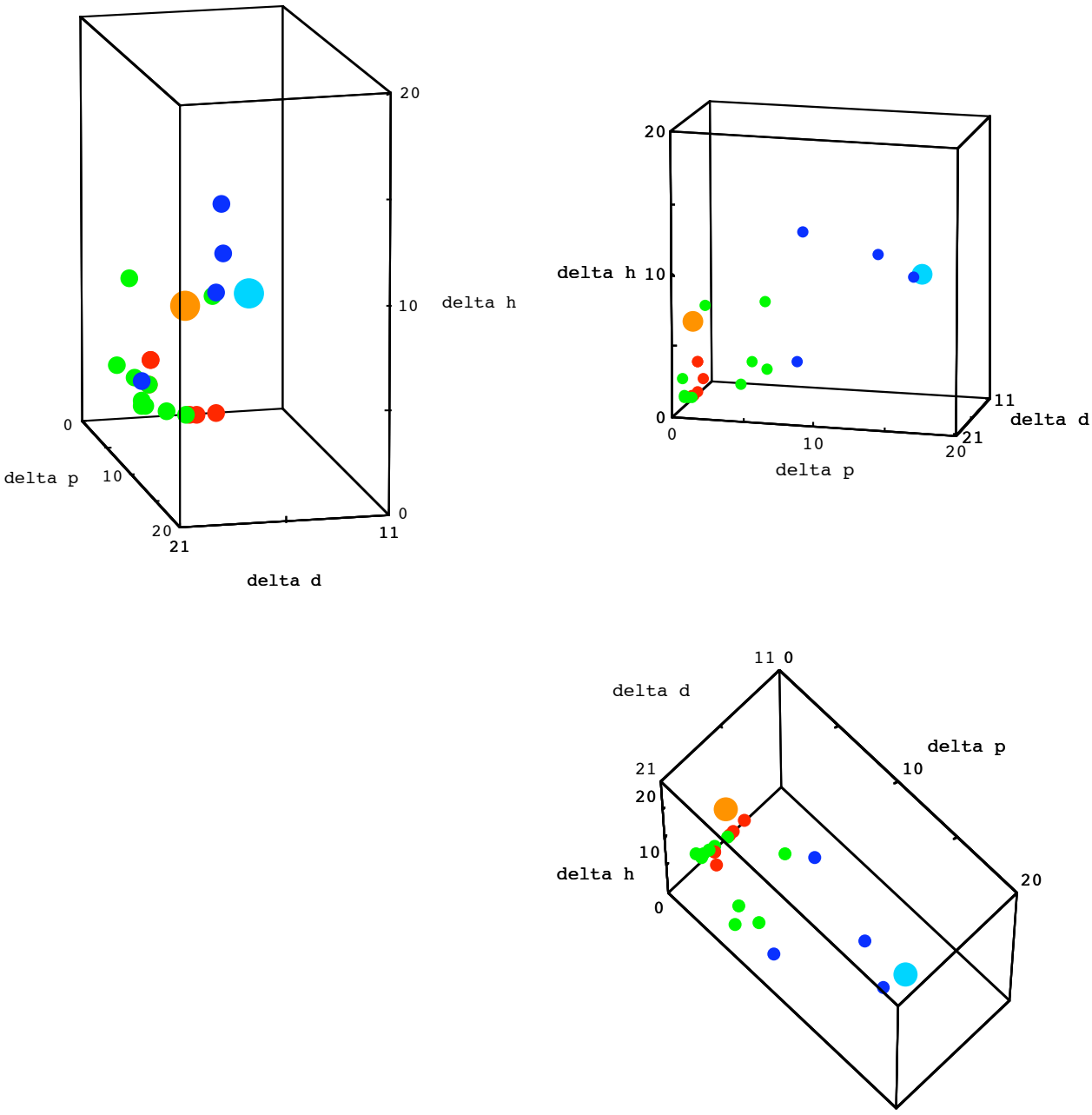

Figure S12. Solubility data for LMWG **6** (< 50g/L, room temperature) represented in Hansen space (Units: $MPa^{0.5}$) (data taken from reference 6). Blue: soluble; red: gel; green: insoluble. Cyan: centre of the solubility sphere; orange: centre of the gelation sphere.

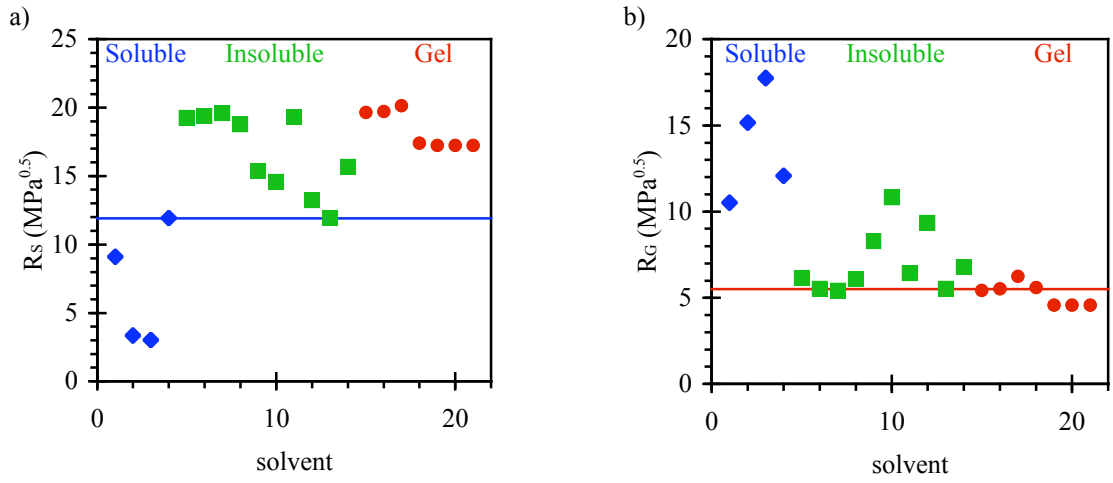

Figure S13. Distances in Hansen space to the centre of the **solubility sphere**[*] [δ_d = 16.9; δ_p = 16.7; δ_h = 10.1; R_{Sol} = 11.9 MPa$^{0.5}$] (a) or to the centre of the **gelation sphere** [δ_d = 15.9; δ_p = 0.1; δ_h = 5.4; R_{Gel} = 5.5 MPa$^{0.5}$] (b) for LMWG **6**. The line represents the radius of the sphere. Blue: soluble; red: gel; green: insoluble.

[*] The location of the solubility sphere is not precise, due to the limited data available (too few good solvents (S)).

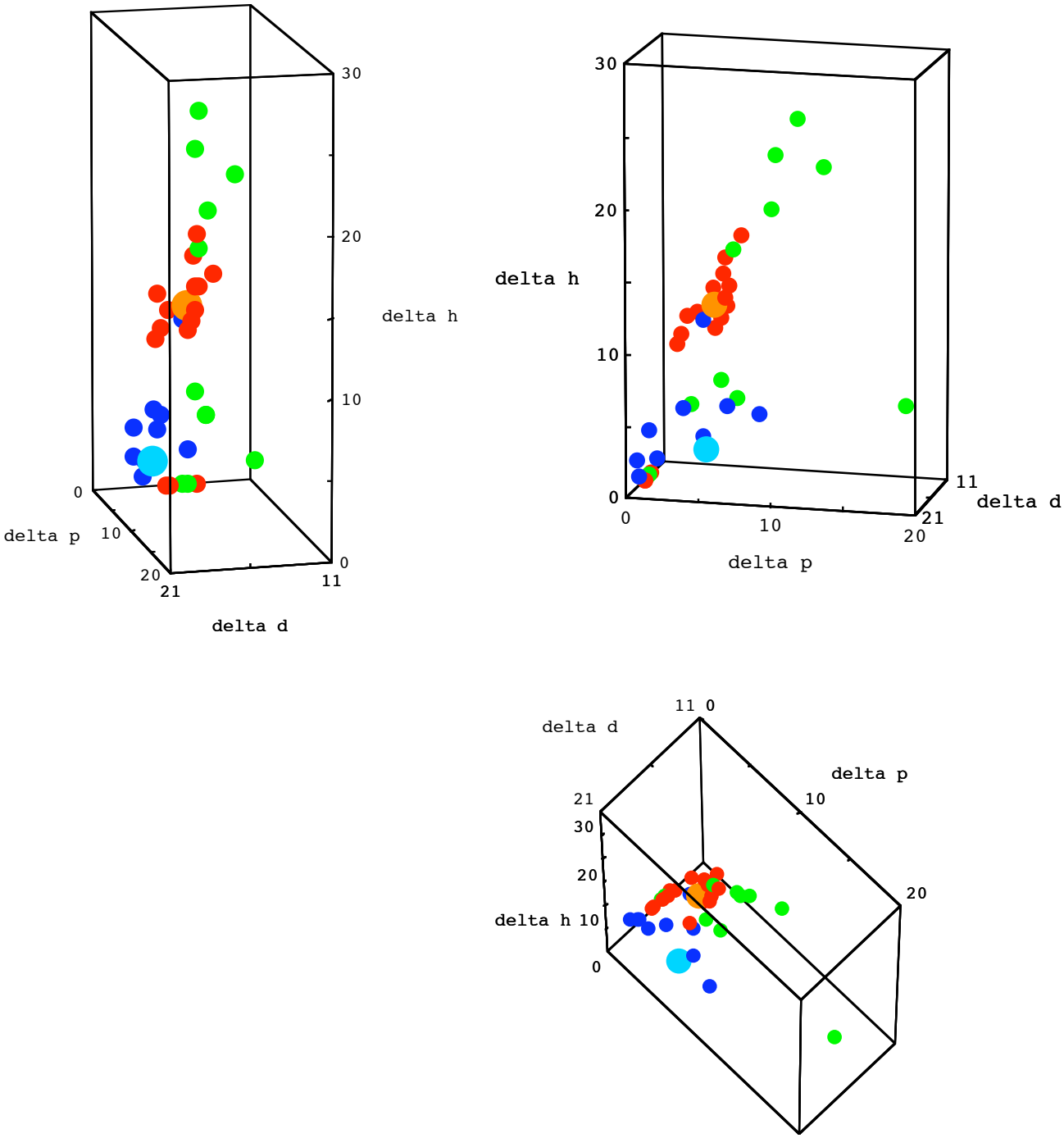

Figure S14. Solubility data for LMWG **7** (20g/L, room temperature) represented in Hansen space (Units: $MPa^{0.5}$) (data taken from reference 7). Blue: soluble; red: gel; green: insoluble. Cyan: centre of the solubility sphere; orange: centre of the gelation sphere.

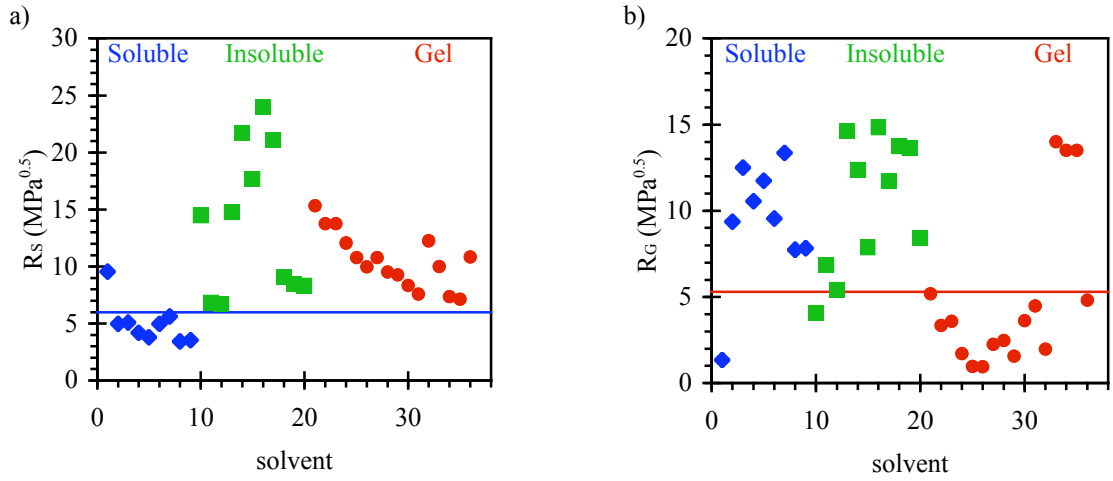

Figure S15. Distances in Hansen space to the centre of the **solubility sphere** [δ_d = 18.4; δ_p = 5.0; δ_h = 2.9; R_{Sol} = 6.0 MPa$^{0.5}$] (a) or to the centre of the **gelation sphere** [δ_d = 16.2; δ_p = 5.0; δ_h = 12.5; R_{Gel} = 5.3 MPa$^{0.5}$] (b) for LMWG **7**. The line represents the radius of the sphere. Blue: soluble; red: gel; green: insoluble.

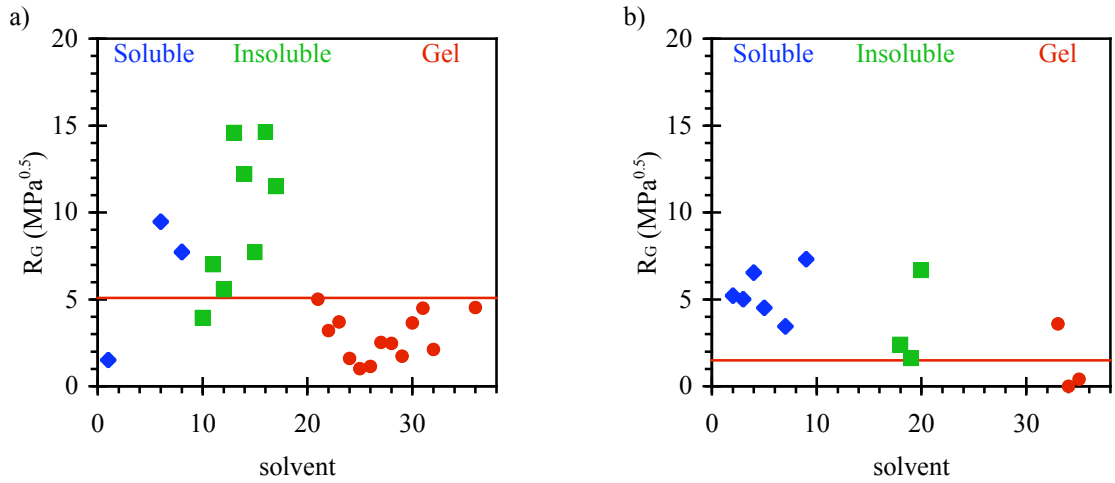

Figure S16. *A better correlation is obtained by considering 2 gelation spheres: the same data as in figure S15b is plotted again. Each solvent is represented only once, either in figure S16a or in figure S16b: only the shortest distance to the gelation sphere centers is considered.* Distances in Hansen space to the centre of the **first gelation sphere** [δ_d = 17.8; δ_p = 0.0; δ_h = 1.2; R_{Gel} = 5.0] (a) or to the centre of the **second gelation sphere** [δ_d = 13.9; δ_p = 4.3; δ_h = 0.6; R_{Gel} = 5.0] (b) for LMWG **7**. The line represents the radius of the sphere. Blue: soluble; red: gel; green: insoluble.

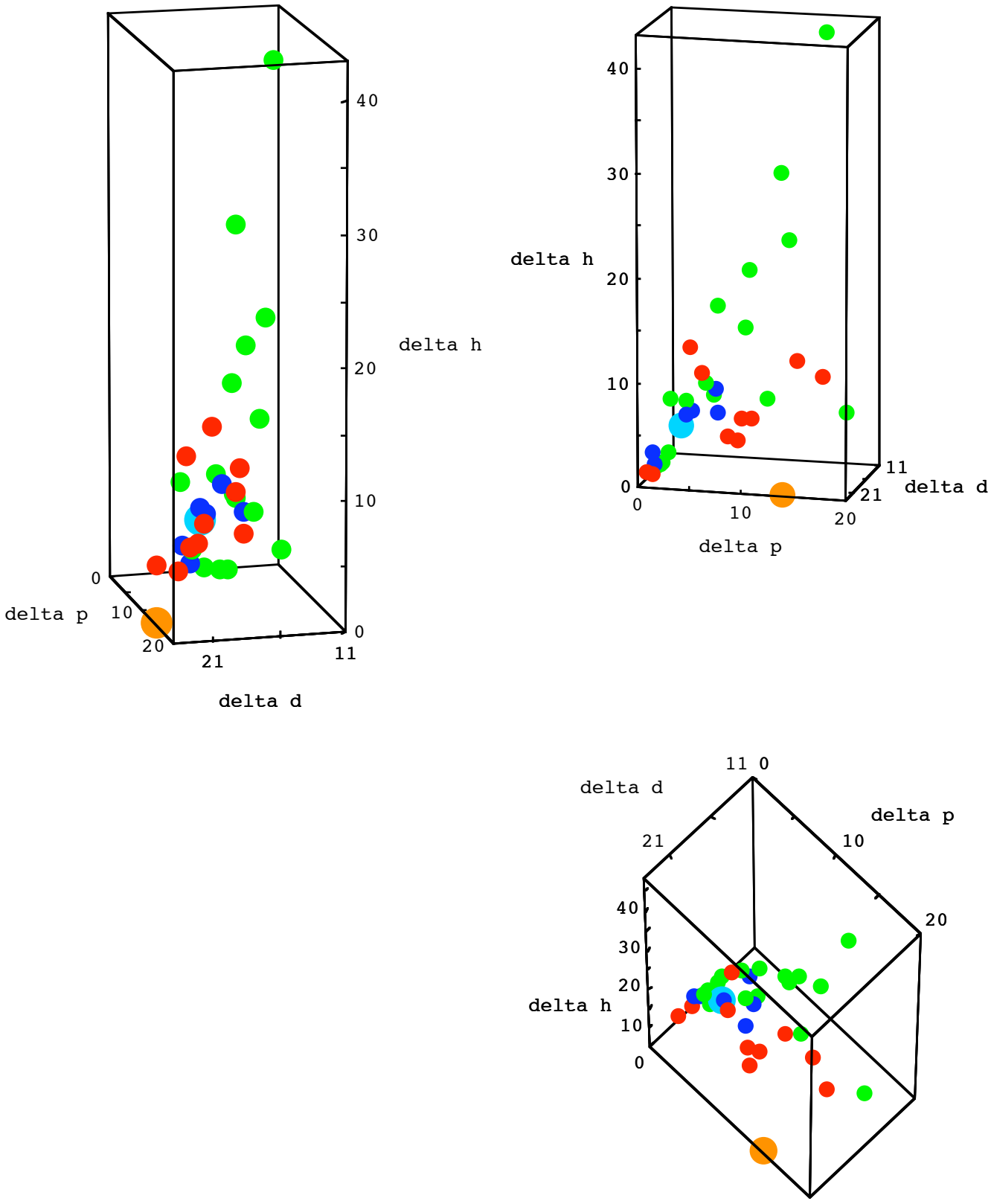

Figure S17. Solubility data for LMWG **8** (< 70g/L, 2-20°C) represented in Hansen space (Units: $MPa^{0.5}$) (data taken from reference 8). Blue: soluble; red: gel; green: insoluble. Cyan: centre of the solubility sphere; orange: centre of the gelation sphere.

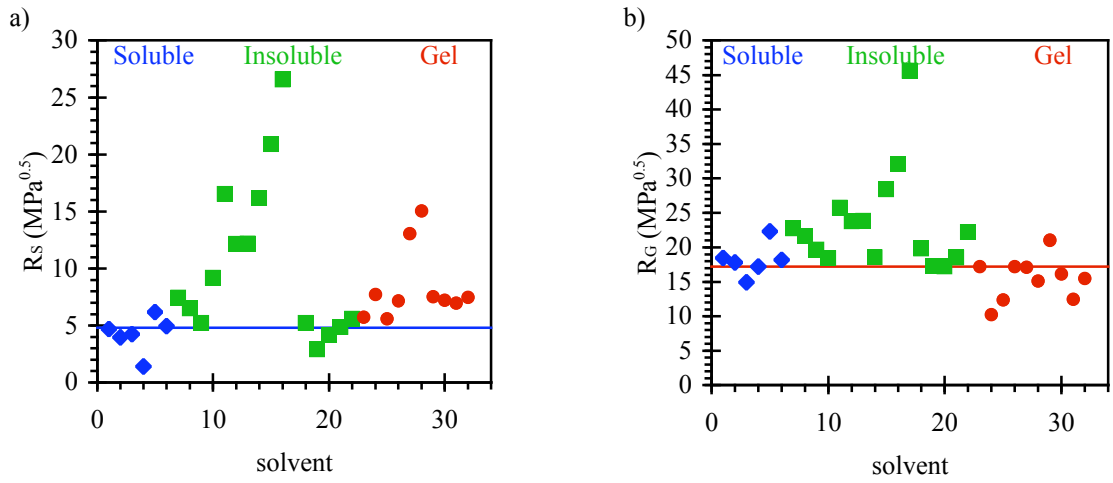

Figure S18. Distances in Hansen space to the centre of the **solubility sphere** [δ_d = 17.6; δ_p = 2.6; δ_h = 4.5; R_{Sol} = 4.8 MPa$^{0.5}$] (a) or to the centre of the **gelation sphere** [δ_d = 23.8; δ_p = 14.0; δ_h = 0.0; R_{Gel} = 17.2 MPa$^{0.5}$] (b) for LMWG **8**. The line represents the radius of the sphere. Blue: soluble; red: gel; green: insoluble.

References

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