Supplementary Material (ESI) for New Journal of Chemistry


# A Low Molecular Weight Hydro and Organogelator Derived from an Isohexide and Sol-gel Transcription of the Alcogel.

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## Supplementary data

Key to tables

| **Key :** | |
|---|---|
| Gel (can invert) | GI |
| Gel (cannot invert) | GN |
| Solution with precipitate | P |
| Crystallisation | C |
| Saturated solution when heating | SS |
| Solution without precipitate | S |

**Table 2.** Sol to Gel Testing of **1** in Water.

| **Gelator (%)** | **Mass Gelator (g)** | **Solvent ($cm^3$)** | **Time to form gel** | **Temp (°C) begin gel** | **Temp (°C) finish gel** | **Key** |
|---|---|---|---|---|---|---|
| 0.1 | 0.006 | 6 | N/A | N/A | N/A | S |
| 0.2 | 0.012 | 6 | N/A | N/A | N/A | S |
| 0.3 | 0.018 | 6 | N/A | N/A | N/A | S |
| 0.4 | 0.024 | 6 | N/A | N/A | N/A | S |
| 0.5 | 0.030 | 6 | N/A | N/A | N/A | S |
| 0.6 | 0.036 | 6 | N/A | N/A | N/A | C |
| 0.7 | 0.042 | 6 | N/A | N/A | N/A | C |
| 0.8 | 0.048 | 6 | N/A | N/A | N/A | C |
| 0.9 | 0.054 | 6 | 19.58 | 36 | 30 | GN |
| 1.0 | 0.060 | 6 | 17.23 | 36 | 31 | GN |
| 1.1 | 0.066 | 6 | 16.15 | 37 | 33 | GN |
| 1.2 | 0.072 | 6 | 15.45 | 38 | 35 | GN |
| 1.3 | 0.078 | 6 | 15.37 | 38 | 35 | GN |
| 1.4 | 0.084 | 6 | 14.41 | 40 | 36 | GN |
| 1.5 | 0.090 | 6 | 13.5 | 40 | 40 | GN |
| 1.6 | 0.096 | 6 | 12.41 | 42 | 39 | GN |
| 1.7 | 0.102 | 6 | 11.2 | 42 | 40 | GN |
| 1.8 | 0.108 | 6 | 9.55 | 44 | 40 | GN |
| 1.9 | 0.114 | 6 | 9.4 | 46 | 42 | GN |
| 2.0 | 0.120 | 6 | 8.01 | 46 | 42 | GI |

**Table 3.** Sol to Gel Testing of **1** in Methanol.

| Percentage Gelator (wt/v) | Mass Gelator (g) | Methanol Quantity ($cm^3$) | Time to form gel (mins) | Temp (°C) begin gel | Temp (°C) finish gel | Key |
|---|---|---|---|---|---|---|
| 0.1 | 0.006 | 6 | N/A | N/A | N/A | S |
| 0.2 | 0.012 | 6 | N/A | N/A | N/A | S |
| 0.3 | 0.018 | 6 | N/A | N/A | N/A | S |
| 0.4 | 0.024 | 6 | N/A | N/A | N/A | S |
| 0.5 | 0.030 | 6 | N/A | 18 | N/A | C |
| 0.6 | 0.036 | 6 | 10.46 | 23 | 19 | GN |
| 0.7 | 0.042 | 6 | 8.51 | 25 | 23 | GN |
| 0.8 | 0.048 | 6 | 7.41 | 25 | 23 | GI |
| 0.9 | 0.054 | 6 | 7.34 | 27 | 25 | GI |
| 1.0 | 0.060 | 6 | 7.01 | 31 | 27 | GI |
| 1.1 | 0.066 | 6 | 7.00 | 27 | 23 | GI |
| 1.2 | 0.072 | 6 | 6.49 | 27 | 24 | GI |
| 1.3 | 0.078 | 6 | 6.21 | 29 | 26 | GI |
| 1.4 | 0.084 | 6 | 6.08 | 36 | 31 | GI |
| 1.5 | 0.090 | 6 | 5.57 | 37 | 31 | GI |
| 1.6 | 0.096 | 6 | 5.40 | 37 | 32 | GI |
| 1.7 | 0.102 | 6 | 5.22 | 37 | 32 | GI |
| 1.8 | 0.108 | 6 | 4.01 | 37 | 32 | GI |
| 1.9 | 0.114 | 6 | 3.56 | 39 | 33 | GI |
| 2.0 | 0.120 | 6 | 3.32 | 40 | 34 | GI |

**Table 4.** Sol to Gel Testing of **1** in Ethanol.

| Percentage Gelator (wt/v) | Mass of gelator (g) | Ethanol Quantity ($cm^3$) | Time taken to form gel (mins) | Temp (°C) begin gel | Temp (°C) finish gel | Key |
|---|---|---|---|---|---|---|
| 0.1 | 0.006 | 6 | N/A | N/A | N/A | C |
| 0.2 | 0.012 | 6 | 11.20 | 26 | 22 | P |
| 0.3 | 0.018 | 6 | 9.09 | 26 | 22 | P |
| 0.4 | 0.024 | 6 | 7.51 | 29 | 23 | GN |
| 0.5 | 0.030 | 6 | 7.12 | 32 | 24 | GI |
| 0.6 | 0.036 | 6 | 7.01 | 35 | 26 | GI |
| 0.7 | 0.042 | 6 | 6.40 | 37 | 27 | GI |
| 0.8 | 0.048 | 6 | 6.34 | 38 | 27 | GI |
| 0.9 | 0.054 | 6 | 6.21 | 39 | 31 | GI |
| 1.0 | 0.060 | 6 | 3.07 | 42 | 38 | GI |
| 1.1 | 0.066 | 6 | 3.09 | 43 | 39.0 | GI |
| 1.2 | 0.072 | 6 | 3.14 | 44.0 | 40.0 | GI |
| 1.3 | 0.078 | 6 | N/A | N/A | N/A | SS |
| 1.4 | 0.084 | 6 | N/A | N/A | N/A | SS |
| 1.5 | 0.090 | 6 | N/A | N/A | N/A | SS |
| 1.6 | 0.096 | 6 | N/A | N/A | N/A | SS |
| 1.7 | 0.102 | 6 | N/A | N/A | N/A | SS |
| 1.8 | 0.108 | 6 | N/A | N/A | N/A | SS |
| 1.9 | 0.114 | 6 | N/A | N/A | N/A | SS |
| 2.0 | 0.120 | 6 | N/A | N/A | N/A | SS |

**Table 5.** Sol to Gel Testing of **1** in 2-Propanol.

| Gelator (%) | Mass Gelator (g) | 2-propanol ($cm^3$) | Time to form gel | Temp (°C) begin gel | Temp (°C) finish gel | Key |
|---|---|---|---|---|---|---|
| 0.1 | 0.006 | 6 | N/A | N/A | N/A | S |
| 0.2 | 0.012 | 6 | 9.41 | 24 | 20 | GN |
| 0.3 | 0.018 | 6 | 9.17 | 24 | 22 | GN |
| 0.4 | 0.024 | 6 | 8.24 | 29 | 27 | GN |
| 0.5 | 0.030 | 6 | 6.50 | 34 | 30 | GN |
| 0.6 | 0.036 | 6 | 6.10 | 36 | 34 | GI |
| 0.7 | 0.042 | 6 | 4.45 | 38 | 35 | GI |
| 0.8 | 0.048 | 6 | 4.01 | 38 | 36 | GI |
| 0.9 | 0.054 | 6 | 3.46 | 39 | 36 | GI |
| 1.0 | 0.060 | 6 | 3.20 | 39 | 37 | GI |
| 1.1 | 0.066 | 6 | N/A | N/A | N/A | SS |
| 1.2 | 0.072 | 6 | N/A | N/A | N/A | SS |
| 1.3 | 0.078 | 6 | N/A | N/A | N/A | SS |
| 1.4 | 0.084 | 6 | N/A | N/A | N/A | SS |
| 1.5 | 0.090 | 6 | N/A | N/A | N/A | SS |
| 1.6 | 0.096 | 6 | N/A | N/A | N/A | SS |
| 1.7 | 0.102 | 6 | N/A | N/A | N/A | SS |
| 1.8 | 0.108 | 6 | N/A | N/A | N/A | SS |
| 1.9 | 0.114 | 6 | N/A | N/A | N/A | SS |
| 2.0 | 0.120 | 6 | N/A | N/A | N/A | SS |

**Table 6.** Sol to Gel Testing of **1** in 1-Butanol.

| Gelator (%) | Mass Gelator (g) | Butanol ($cm^3$) | Time to form gel | Temp (°C) begin gel | Temp (°C) finish gel | Key |
|---|---|---|---|---|---|---|
| 0.1 | 0.006 | 6 | N/A | N/A | N/A | S |
| 0.2 | 0.012 | 6 | N/A | N/A | N/A | S |
| 0.3 | 0.018 | 6 | N/A | N/A | N/A | S |
| 0.4 | 0.024 | 6 | N/A | N/A | N/A | S |
| 0.5 | 0.030 | 6 | N/A | N/A | N/A | S |
| 0.6 | 0.036 | 6 | 17.55 | 32 | 29 | GN |
| 0.7 | 0.042 | 6 | 17.50 | 32 | 30 | GN |
| 0.8 | 0.048 | 6 | 14.17 | 33 | 30 | GI |
| 0.9 | 0.054 | 6 | 12.41 | 34 | 30 | GI |
| 1.0 | 0.060 | 6 | 12.32 | 37 | 32 | GI |
| 1.1 | 0.066 | 6 | 11.35 | 37 | 33 | GI |
| 1.2 | 0.072 | 6 | 10.29 | 38 | 33 | GI |
| 1.3 | 0.078 | 6 | 10.04 | 40 | 36 | GI |
| 1.4 | 0.084 | 6 | N/A | N/A | N/A | SS |
| 1.5 | 0.090 | 6 | N/A | N/A | N/A | SS |
| 1.6 | 0.096 | 6 | N/A | N/A | N/A | SS |
| 1.7 | 0.102 | 6 | N/A | N/A | N/A | SS |
| 1.8 | 0.108 | 6 | N/A | N/A | N/A | SS |
| 1.9 | 0.114 | 6 | N/A | N/A | N/A | SS |
| 2.0 | 0.120 | 6 | N/A | N/A | N/A | SS |

**Table 7.** Sol to Gel Testing of **1** in Toluene.

| Gelator (%) | Mass Gelator (g) | Toluene ($cm^3$) | Time to form gel | Temp (°C) begin gel | Temp (°C) finish gel | Key |
|---|---|---|---|---|---|---|
| 0.1 | 0.006 | 6 | N/A | N/A | N/A | S |
| 0.2 | 0.012 | 6 | N/A | N/A | N/A | S |
| 0.3 | 0.018 | 6 | N/A | N/A | N/A | S |
| 0.4 | 0.024 | 6 | N/A | N/A | N/A | S |
| 0.5 | 0.030 | 6 | N/A | N/A | N/A | S |
| 0.6 | 0.036 | 6 | 15.34 | 30 | 23 | GN |
| 0.7 | 0.042 | 6 | 12.55 | 30 | 25 | GN |
| 0.8 | 0.048 | 6 | 11.18 | 32 | 27 | GN |
| 0.9 | 0.054 | 6 | 10.56 | 32 | 28 | GN |
| 1.0 | 0.060 | 6 | 9.49 | 32 | 28 | GN |
| 1.1 | 0.066 | 6 | 9.12 | 34 | 29 | GN |
| 1.2 | 0.072 | 6 | 8.51 | 34 | 30 | GI |
| 1.3 | 0.078 | 6 | 8.42 | 34 | 30 | GI |
| 1.4 | 0.084 | 6 | 8.17 | 35 | 33 | GI |
| 1.5 | 0.090 | 6 | 8.03 | 38 | 35 | GI |
| 1.6 | 0.096 | 6 | 7.34 | 39 | 37 | GI |
| 1.7 | 0.102 | 6 | 6.56 | 40 | 38 | GI |
| 1.8 | 0.108 | 6 | 6.26 | 42 | 38 | GI |
| 1.9 | 0.114 | 6 | N/A | N/A | N/A | SS |
| 2.0 | 0.120 | 6 | N/A | N/A | N/A | SS |

**Table 8.** Sol to Gel Testing of **1** in Benzene.

| Gelator (%) | Mass Gelator (g) | Benzene ($cm^3$) | Time to form gel | Temp (°C) begin gel | Temp (°C) finish gel | Key |
|---|---|---|---|---|---|---|
| 0.1 | 0.006 | 6 | N/A | N/A | N/A | S |
| 0.2 | 0.012 | 6 | N/A | N/A | N/A | S |
| 0.3 | 0.018 | 6 | N/A | N/A | N/A | S |
| 0.4 | 0.024 | 6 | 21.32 | 30 | 27 | GN |
| 0.5 | 0.030 | 6 | 20.51 | 33 | 29 | GN |
| 0.6 | 0.036 | 6 | 19.18 | 34 | 29 | GN |
| 0.7 | 0.042 | 6 | 19.35 | 34 | 29 | GI |
| 0.8 | 0.048 | 6 | 14.22 | 35 | 30 | GI |
| 0.9 | 0.054 | 6 | 12.53 | 35 | 32 | GI |
| 1.0 | 0.060 | 6 | 10.5 | 36 | 32 | GI |
| 1.1 | 0.066 | 6 | 10.31 | 37 | 35 | GI |
| 1.2 | 0.072 | 6 | 10.04 | 37 | 34 | GI |
| 1.3 | 0.078 | 6 | 9.37 | 37 | 35 | GI |
| 1.4 | 0.084 | 6 | 7.55 | 38 | 36 | GI |
| 1.5 | 0.090 | 6 | 7.53 | 38 | 36 | GI |
| 1.6 | 0.096 | 6 | 7.03 | 38 | 36 | GI |
| 1.7 | 0.102 | 6 | 6.44 | 40 | 38 | GI |
| 1.8 | 0.108 | 6 | 6.31 | 41 | 38 | GI |
| 1.9 | 0.114 | 6 | 4.51 | 44 | 39 | GI |
| 2.0 | 0.120 | 6 | 4.2 | 44 | 40 | GI |

**Table 9.** Gel to sol Testing of **1** in Water.

| Percentage Gelator | Mass of 2 (g) | Solvent Quantity ($cm^3$) | Temperature at Gel - Sol (°C) |
|---|---|---|---|
| 2.0 | 0.120 | 6 | 86 |

**Table 10.** Gel to sol Testing of **1** in Methanol.

| Percentage Gelator | Mass of 2 (g) | Solvent Quantity ($cm^3$) | Temperature at Gel - Sol (°C) |
|---|---|---|---|
| 0.8 | 0.048 | 6 | 61 |
| 0.9 | 0.054 | 6 | 63 |
| 1.0 | 0.060 | 6 | 63 |
| 1.1 | 0.066 | 6 | 64 |
| 1.2 | 0.072 | 6 | 65 |
| 1.3 | 0.078 | 6 | 69 |
| 1.4 | 0.084 | 6 | 72 |
| 1.5 | 0.090 | 6 | 73 |
| 1.6 | 0.096 | 6 | 76 |
| 1.7 | 0.102 | 6 | 77 |
| 1.8 | 0.108 | 6 | 79 |
| 1.9 | 0.114 | 6 | 80 |
| 2.0 | 0.120 | 6 | 82 |

**Table 11.** Gel to sol Testing of **1** in Ethanol.

| Percentage Gelator | Mass of 2 (g) | Solvent Quantity ($cm^3$) | Temperature at Gel - Sol (°C) |
|---|---|---|---|
| 0.5 | 0.030 | 6 | 66 |
| 0.6 | 0.036 | 6 | 68 |
| 0.7 | 0.042 | 6 | 70 |
| 0.8 | 0.048 | 6 | 71 |
| 0.9 | 0.054 | 6 | 76 |
| 1.0 | 0.060 | 6 | 85 |
| 1.1 | 0.066 | 6 | 86 |
| 1.2 | 0.072 | 6 | 89 |

**Table 12.** Gel to sol Testing of **1** in 2-Propanol.

| Percentage Gelator | Mass of 2 (g) | Solvent Quantity ($cm^3$) | Temperature at Gel - Sol (°C) |
|---|---|---|---|
| 0.6 | 0.036 | 6 | 61 |
| 0.7 | 0.042 | 6 | 65 |
| 0.8 | 0.048 | 6 | 67 |
| 0.9 | 0.054 | 6 | 70 |
| 1.0 | 0.060 | 6 | 73 |

**Table 13.** Gel to sol Testing of **1** in 1-Butanol.

| Percentage Gelator | Mass of 2 (g) | Solvent Quantity ($cm^3$) | Temperature at Gel - Sol (°C) |
|---|---|---|---|
| 0.8 | 0.048 | 6 | 71 |
| 0.9 | 0.054 | 6 | 74 |
| 1.0 | 0.060 | 6 | 77 |
| 1.1 | 0.066 | 6 | 78 |
| 1.2 | 0.072 | 6 | 80 |
| 1.3 | 0.078 | 6 | 81 |

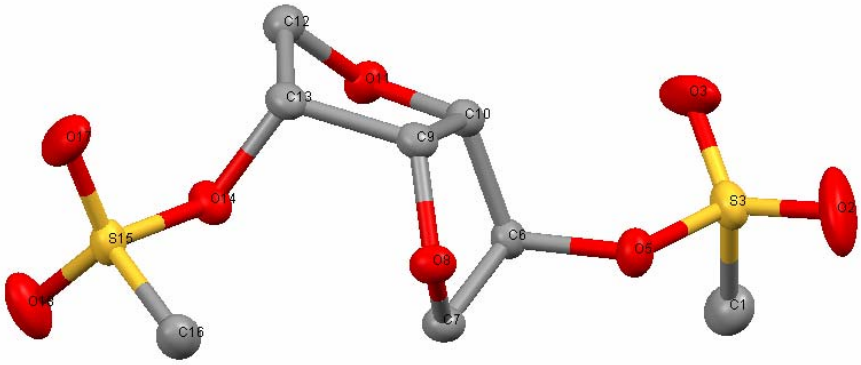
**Table 14.** Gel to sol Testing of **1** in Toluene.

| Percentage Gelator | Mass of 2 (g) | Solvent Quantity ($cm^3$) | Temperature at Gel - Sol (°C) |
|---|---|---|---|
| 1.2 | 0.072 | 6 | 67 |
| 1.3 | 0.078 | 6 | 68 |
| 1.4 | 0.084 | 6 | 71 |
| 1.5 | 0.090 | 6 | 74 |
| 1.6 | 0.096 | 6 | 75 |
| 1.7 | 0.102 | 6 | 76 |
| 1.8 | 0.108 | 6 | 81 |

**Table 15.** Gel to sol Testing of **1** in Benzene.

| Percentage Gelator | Mass of 2 (g) | Solvent Quantity ($cm^3$) | Temperature at Gel - Sol (°C) |
|---|---|---|---|
| 0.7 | 0.042 | 6 | 65 |
| 0.8 | 0.048 | 6 | 66 |
| 0.9 | 0.054 | 6 | 66 |
| 1.0 | 0.060 | 6 | 66 |
| 1.1 | 0.066 | 6 | 67 |
| 1.2 | 0.072 | 6 | 67 |
| 1.3 | 0.078 | 6 | 71 |
| 1.4 | 0.084 | 6 | 72 |
| 1.5 | 0.090 | 6 | 72 |
| 1.6 | 0.096 | 6 | 72 |
| 1.7 | 0.102 | 6 | 74 |
| 1.8 | 0.108 | 6 | 75 |
| 1.9 | 0.114 | 6 | 76 |
| 2.0 | 0.120 | 6 | 79 |

**The Structural Data for 2,5-di-*O*-methanesulfonyl-1,4:3,6-dianhydro-D-sorbitol (1) from Single Crystal X-Ray Crystallography**




**Thermal ellipsoids are at 30 % probability and H's are removed for clarity. $C_8H_{14}O_8S_2$: orthorhombic, space group $P2_12_12_1$, $a$ = 5.4647(8), $b$ = 11.1834(17), $c$ = 20.479(3), $V$ = 1251.55 Å, $T$ = 298(2) K, Z = 4, $\mu$(Mo-$K_\alpha$) = 0.929 mm$^{-1}$, 2209 independent reflections measured, $d_{calc}$ = 1.604 gcm$^{-3}$, $R_1$ = 0.0291, $wR_2$ = 0.0693 and 165 refined parameters, CCD = 646818.**

**Selected Bond Distances and Angles:**

| | | | |
|---|---|---|---|
| C(1)–S(3) | 1.742(3) | C(10)–O(11) | 1.429(3) |
| O(2)–S(3) | 1.408(2) | O(11)–C(12) | 1.434(3) |
| S(3)–O(3) | 1.416(2) | C(13)–O(14) | 1.460(3) |
| S(3)–O(5) | 1.5770(18) | O(14)–S(15) | 1.5769(17) |
| O(5)–C(6) | 1.460(3) | S(15)–O(18) | 1.4120(19) |
| C(7)–O(8) | 1.429(3) | S(15)–O(17) | 1.4264(19) |
| O(8)–C(9) | 1.431(3) | S(15)–C(16) | 1.746(2) |
| O(11)–C(10)–C(6) | 109.16(18) | C(13)–O(14)–S(15) | 121.94(14) |
| O(8)–C(9)–C(13) | 114.54(18) | O(5)–S(3)–C(1) | 104.67(12) |
| O(5)–C(6)–C(10) | 110.20(17) | O(2)–S(3)–O(5) | 103.92(14) |
| O(5)–C(6)–C(7) | 106.34(18) | O(3)–S(3)–O(5) | 109.38(10) |
| O(14)–C(13)–C(9) | 109.90(18) | O(14)–S(15)–C(16) | 104.32(11) |
| O(14)–C(13)–C(12) | 106.14(19) | O(18)–S(15)–O(14) | 104.00(11) |
| C(6)–O(5)–S(3) | 119.22(14) | O(17)–S(15)–O(14) | 108.96(11) |