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SUPPORTING INFORMATION

Title: Tripodal Tris-Urea Derivatives as Gelators for Organic Solvents

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¹H NMR spectra were recorded on a Varian Gemini-200 (200 MHz) or a Varian VXR-300 (300 MHz) spectrometer. Chemical shifts are denoted in δ-units (ppm) relative to residual solvent peaks (CDCl₃, δ = 7.26; DMSO-d₆, δ = 2.49). ¹³C NMR spectra were recorded on a Varian Gemini-200 (50.32 MHz) or a Varian VXR-300 (75.48 MHz) spectrometer. Chemical shifts are denoted in δ-units (ppm) relative to the solvent (CDCl₃, δ = 76.91; DMSO-d₆, δ = 39.5) and converted to the TMS scale.

General procedure for the synthesis of 1-7.

To a solution of tris(2-aminoethyl) amine (1 eqv.) in CHCl₃ was added the corresponding isocyanate (3 eqv.) in CHCl₃. After stirring for 2 hours the solvent was evaporated *in vacuo* and the remaining white solid was stirred in diethyl ether, filtered off and eventually recrystallised from CHCl₃. Conversion was complete.

1: ¹H NMR (DMSO-d₆): δ = 8.50 (s, 3H), 7.36 (d, 6H, J=7.69 Hz), 7.18 (t, 6H, J=8.87 Hz), 6.86 (t, 3H, J=7.33 Hz), 6.16 (m, 3H), 3.17 (m, 6H), 2.58 (t, 6H, J=6.41 Hz); ¹³C NMR (DMSO-d₆): δ = 155.28, 140.42, 128.56, 120.97, 117.70, 53.92, 37.50; CI: 504 (M + H⁺).

2: ¹H NMR (DMSO-d₆): δ = 9.39 (s, 3H), 8.108 (d, 6H, J=9.52 Hz), 7.58 (d, 6H, J=9.52 Hz), 6.47 (s, 3H), 3.21 (m, 6H), 2.62 (m, 6H); ¹³C NMR (DMSO-d₆): δ = 154.48, 147.17, 140.32, 125.06, 116.77, 53.48, 37.56. C₁₈H₃₀N₁₀O₉

3: ¹H NMR (DMSO-d₆): δ = 7.32-7.18 (m, 15H), 6.44 (t, 3H, J=5.86 Hz), 6.02 (m, 3H), 4.19 (d, 6H, J=5.49 Hz), 3.08 (d, 6H, J=5.50 Hz), 2.49 (d, 6H, J=6.23 Hz); ¹³C NMR (DMSO-d₆): δ = 158.16, 140.82, 128.14, 126.92, 126.45, 54.31, 42.90, 37.78; IR (KBr): ν = 1627, 1579 cm⁻¹; CI: 546 (M + H⁺). C₃₀H₃₉N₇O₃: calcd. C 66.03, H 7.20, N 17.97; found: C 65.9, H 7.23, N 18.01.

4: ¹H NMR (CDCl₃): δ = 6.18 (s, 3H), 5.62 (s, 3H), 3.13-3.07 (m, 12H), 2.48 (m, 6H), 1.48-1.28 (m, 12H), 0.89 (t, 9H, J=7.14 Hz); ¹³C NMR (CDCl₃): δ = 159.68, 55.06, 39.99, 38.37, 32.48, 20.09, 13.79; IR (KBr): ν = 1630, 1585 cm⁻¹; C₂₁H₄₅N₇O₃: calcd. C 56.86, H 10.22, N 22.10; found: C 56.78, H 10.17, N 22.10.

5: ¹H NMR (CDCl₃): δ = 6.06 (s, 3H), 5.54 (s, 3H), 3.09 (m, 12H), 2.46 (s, 6H), 1.44 (m, 6H), 1.25 (s, 30H), 0.85 (t, 9H, J=6.95 Hz); ¹³C NMR (CDCl₃): δ = 159.63, 54.97, 40.47, 38.40, 31.76, 30.52, 29.48, 29.32, 27.12, 22.55, 14.06.

6: ^1H NMR (CDCl_3): $\delta = 5.96$ (s, 3H), 5.45 (s, 3H), 3.10 (m, 12H), 2.47 (s, 6H), 1.44 (m, 6H), 1.23 (s, 54H), 0.85 (t, 6H, $J=6.22$ Hz); ^{13}C NMR (CDCl_3): $\delta = 159.48, 54.87, 40.41, 38.30, 31.83, 30.42, 29.63, 29.47, 29.29, 27.04, 22.59, 13.99$; $\text{C}_{45}\text{H}_{93}\text{N}_7\text{O}_3$: calcd. C 69.27, H 12.01, N 12.57; found: C 69.23, H 12.02, N 12.41.

7: ^1H NMR (DMSO-d_6): $\delta = 5.78$ (t, 3H, $J=5.49$ Hz), 5.64 (d, 3H, $J=8.69$ Hz), 3.41 (m, 3H), 3.00 (m, 6H), 2.41 (t, 6H, 6.22 Hz), 1.41-1.22 (m, 24H), 0.81 (m, 18H); ^{13}C NMR (DMSO-d_6): $\delta = 158.12, 54.61, 49.89, 37.72, 34.29, 27.90, 27.67, 22.17, 13.93, 10.08$; IR (KBr): $\nu = 1628, 1574$ cm^{-1} ; $\text{C}_{30}\text{H}_{63}\text{N}_7\text{O}_3$.

Crystal structure determination of 1.

$\text{C}_{27}\text{H}_{33}\text{N}_7\text{O}_3$, $M_r = 503.60$, colourless, block-shaped crystal (0.2 x 0.3 x 0.3 mm), monoclinic, space group $\text{P}2_1/c$ (no. 14) with $a = 12.4748(12)$, $b = 17.761(3)$, $c = 13.4073(10)$ Å, $\beta = 117.304(7)^\circ$, $V = 2639.6(6)$ Å³, $Z = 4$, $D_x = 1.267$ g cm⁻³, $F(000) = 1072$, $\mu(\text{Mo K}\alpha) = 0.086$ mm⁻¹. 14467 reflections measured, 5958 independent, $R_{int} = 0.0558$, ($1.6^\circ < \theta < 27.4^\circ$, $T = 150$ K, Mo $K\alpha$ radiation, graphite monochromator, $\lambda = 0.71073$ Å) on a Nonius KappaCCD diffractometer on rotating anode. The structure was solved by automated direct methods (SHELXS97 [a]). Refinement on F^2 was carried out by full-matrix least-squares techniques (SHELXL-97 [b]). Hydrogen atoms were located on a difference Fourier map; their coordinates were included as parameters in the refinement. Refinement of 433 parameters converged at a final $wR2$ value of 0.1145, $w = 1/[\sigma^2(F^2) + (0.0438P)^2 + 0.39P]$, where $P = (\text{Max}(F^2_o, 0) + 2F^2_c)/3$, $R1 = 0.0480$ (for 4059 reflections with $I > 2\sigma(I)$), $S = 1.032$, $-0.19 < \Delta\rho < 0.19$ e Å⁻³. Scattering factors were taken from the International Tables for Crystallography [c].

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[b] Sheldrick, G. M. SHELXL-97 Program for crystal structure determination. University of Göttingen, Germany, **1997**.

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