

Supporting Information

Glutamic Acid Dendrimers Attached to a Central Ferrocene Core: Synthesis and Properties.

Francis F. Appoh, Donald S. Thomas and Heinz-Bernhard Kraatz*

Department of Chemistry, University of Saskatchewan, 110 Science Place, Saskatoon, SK S7N 5C9, Canada. Fax: +1-306-966-4730; Tel: +1-306-966-4660; E-mail: kraatz@sask.usask.ca

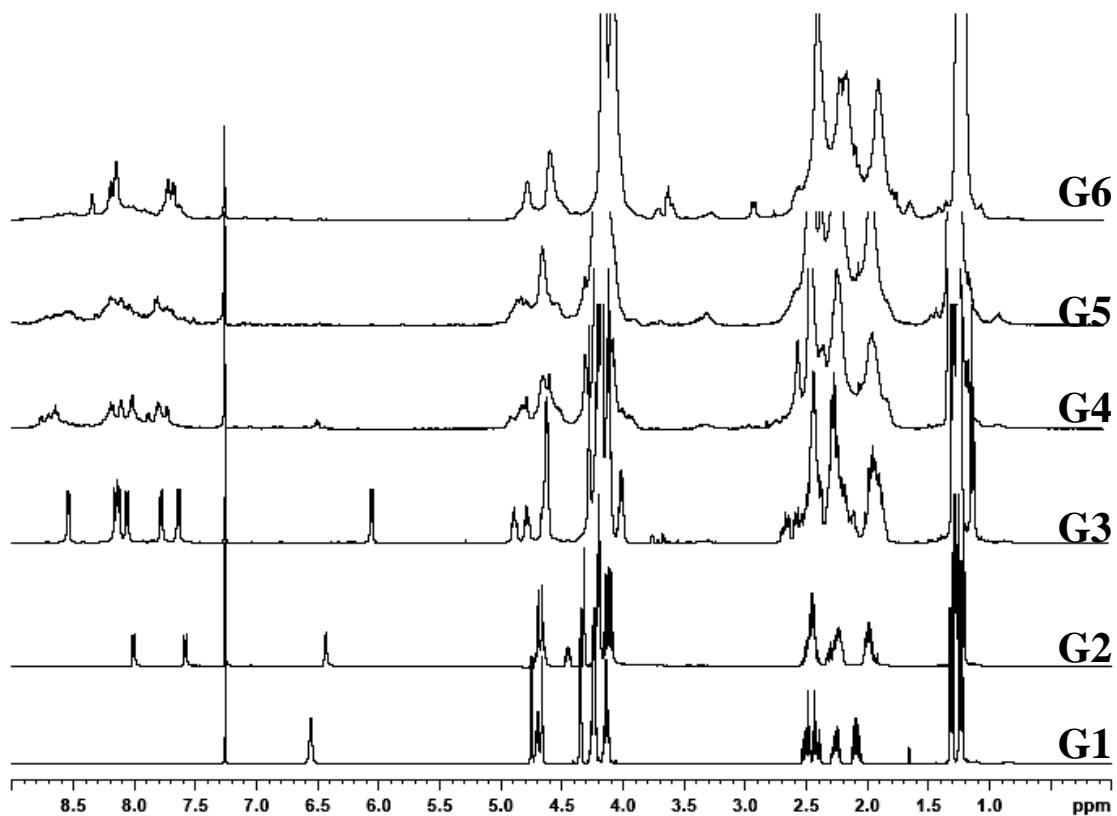


Figure S1. ¹H NMR spectra of G1 - G6 in CDCl₃.

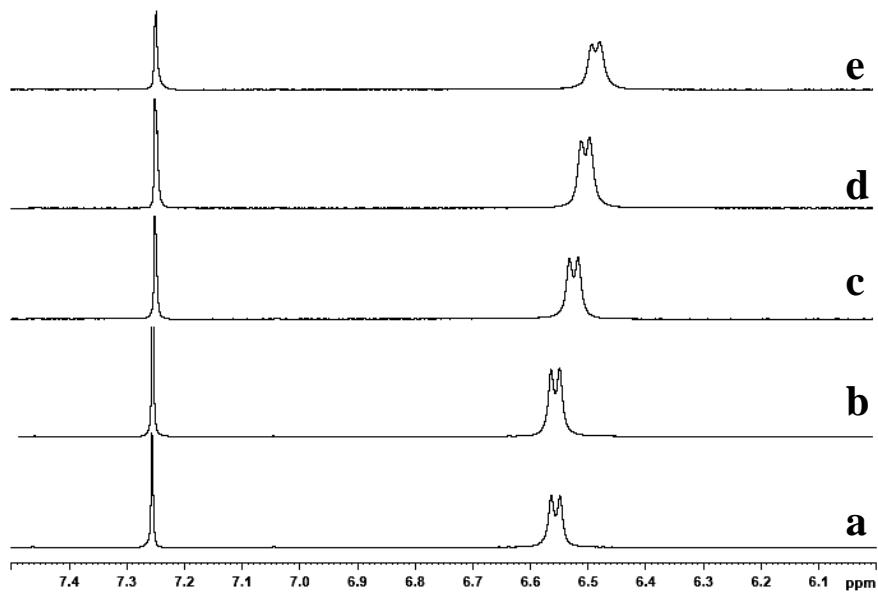


Figure S2 Partial ¹H-NMR spectrum of **G1** in CDCl₃ showing the temperature dependence of the amide chemical shift. (a) 298K (b) 305K (c) 310K(d) 315K (e) 320K.

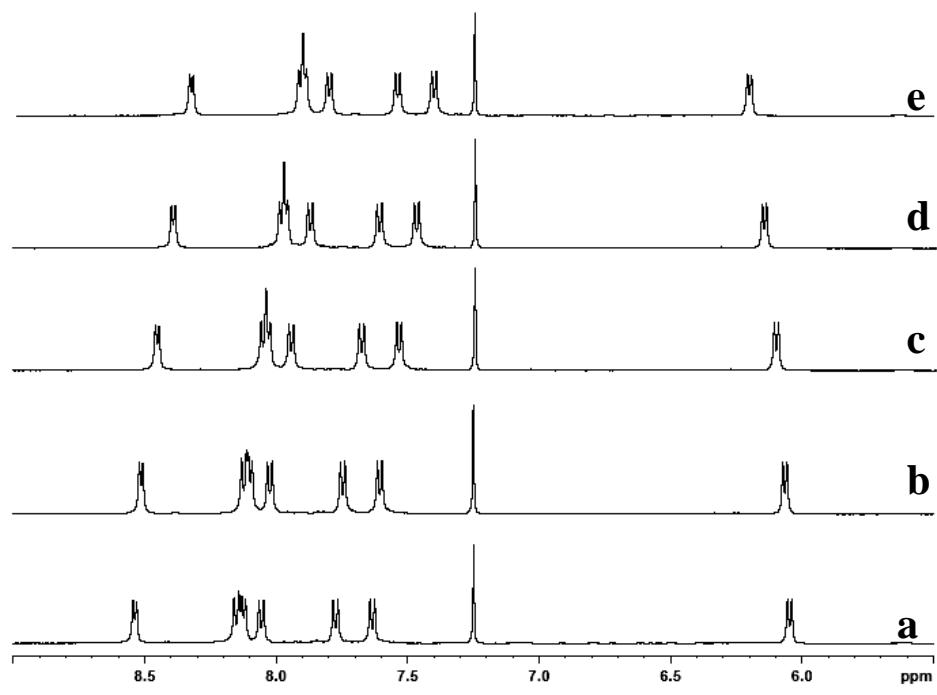


Figure S3 Partial ¹H-NMR spectrum of **G3** in CDCl₃ showing the temperature dependence of the amide chemical shift.. (a) 298K (b) 305K (c) 310K(d) 315K (e) 320K.

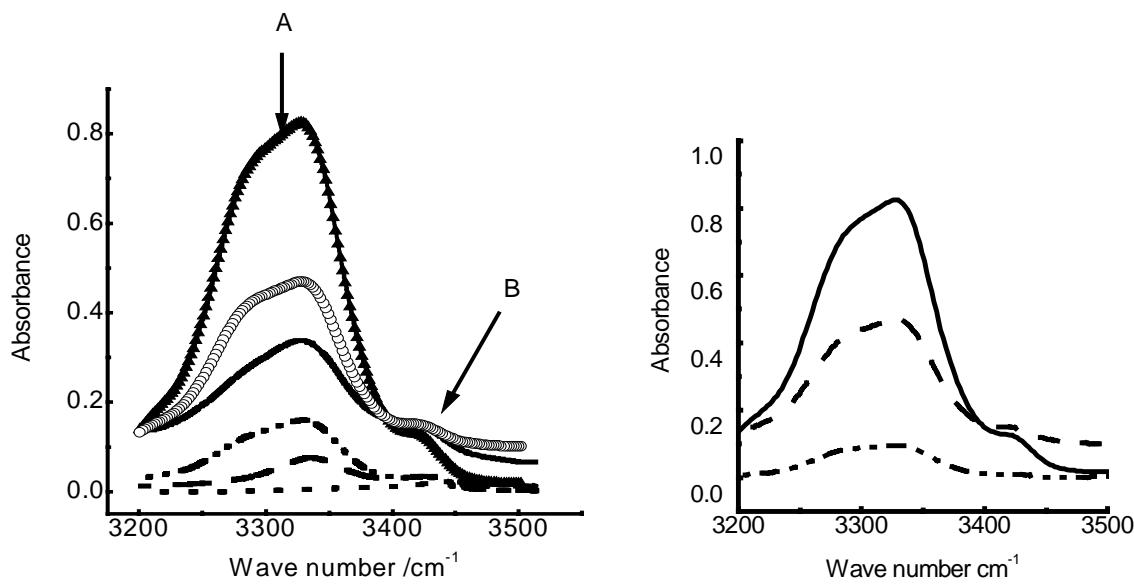


Figure S4 FT-IR showing (left) H-bonded amide NH (A), non-H bonded amide NH (B), of **G1**(●), **G2**(—), **G3**(—●—), **G4**(—), **G5** (○) and **G6** (▲). Right: concentration dependence of **G6** at 1mM (—●—), 5mM (— —) and 10 mM (—)

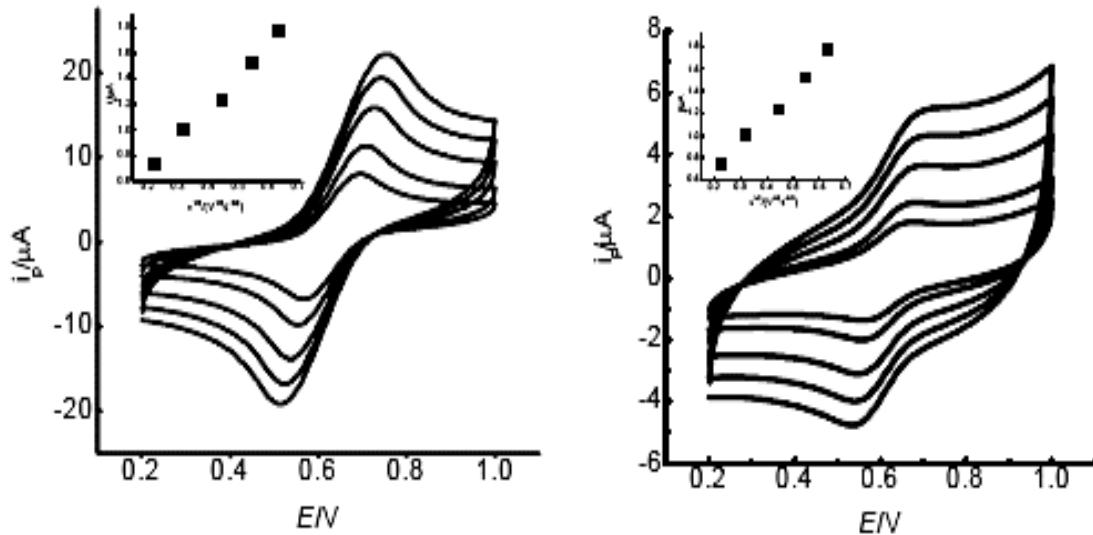


Figure S5 CV (A) of **G1**, (B) **G6** , 0.5 mM Fc-glutamic esters dendrimers at Glassy Carbon Electrode, 0.2 M TBAP supporting electrolyte 50, 100, 200, 300, 400mV·s⁻¹ at 23 ± 1 °C

The diffusion coefficient, D_o , was calculated from the Randles-Sevcik equation. where D_o is the diffusion coefficient in cm²/s and v is the sweep rate in volts/s, A is the area of the electrode, n is the number of electrons and C_o is the bulk concentration of the redox active material. The plotted peak current verses square root scan rate (inset Figure S6) were generally linear over the scan rate used.

$$i_p = (2.69 \times 105) n^{3/2} A D_o^{1/2} v^{1/2} C_o. \quad (2)$$

Table S1. Selected ^1H NMR (ppm) and ^{13}C NMR (ppm) spectra in CDCl_3 , FT-IR (KBr, cm^{-1} , resolution 4cm^{-1}).

	G1	G2	G3	G4	G5	G6
H-Fc	4.25, 4.354, 4.66, 4.75	4.19, 4.32, 4.66, 4.70	4.14, 4.60	4.26, 4.10, 4.23, 4.58	4.16, 4.20, 4.30	--
NH	6.55	8.10, 7.69, 6.40	8.60, 8.23, 8.20, 8.14, 7.85, 7.72, 6.02	8.75, 8.69, 8.63(2H), 8.17(2H), 8.09(2H), 8.00(2H), 7.89, 7.77 (2H), 7.69, 6.48	8.99-7.28	8.98-7.68
C-Cp	75.6, 70.9, 70.1, 68.5	75.6, 71.0, 70.2, 68.7	75.9, 70.7, 70.1, 68.6	77.0, 70.7, 70.1, 68.4	69.7, 69.6, 68.0	-
COO	173.6, 172.3, 170.2.	174.0, 173.2, 172.9, 170.6.	173.9, 174.6, 174.4, 173.0, 174.3, 174.1, 172.6, 174.0, 173.9, 170.6.	175.6, 175.4, 174.7, 174.5, 174.3, 173.7, 173.5, 173.3, 173, 173.6, 173.1, 172.9, 172.8, 172.9, 172.3, 172.5, 172.3, 169.7.	173.8, 173.4, 172.4, 172.6, 172.2, 171.0, 170.0	174.3, 174.1, 174.0, 173.9, 173.8, 173.4, 173.0, 172.7, 172.6, 172.5, 172.4, 172.3,
ν-N-H	3344	3302	3292	3303	3289	3291
ν-(COOR)	1746	1737	1736	1735	1736	1737
ν(CO)	1640	1643	1642	1647	1656, 1642	1657, 1641
ν(C(O)NR)	1547	1535	1535	1541	1544, 1536	1546, 1535
ν(C-H)C_p	3101	3086	3081	3076	3072	3071

Table S2. Data of VT-NMR ($\Delta\delta\text{NH}/\Delta T$; ppb·K-1)^a for 1 mM and 50 mM of **G1 - G4** in CDCl_3 and ($\Delta\delta$ ppm)^b in 20% DMSO-d₆/ CDCl_3 (10 mM).

	G1			G2			G3			G4		
NH	1 mM ^a	50mM ^a	$\Delta\delta$ ppm ^b	1 mM ^a	50mM ^a	$\Delta\delta$ ppm ^b	1 mM ^a	50mM ^a	$\Delta\delta$ ppm ^b	1 mM ^a	50mM ^a	$\Delta\delta$ ppm ^b
1	-4.7	-4.4	0.4	8.3	7.9	0.7	9.6	9.7	0.8	1.1	1.2	0.2
2				-15.6	-15.4	-0.1	-12.8	-12.9	-0.3	-5.6	-5.9	-0.2
3				-11.5	-11.3	-0.1	-13.2	-13.0	-0.4	nd	nd	nd
4							-13.7	-13.9	-0.3	nd	nd	nd
5							-12.7	-12.9	-0.2	nd	nd	nd
6							-13.5	-13.5	-0.4	nd	nd	nd
7							-11.6	-11.7	-0.5	nd	nd	nd
14										-2.7	-5.9	-0.5
15										-0.6	-7.2	-0.2
nd (not determined)												

Determination of Diameter of dendrimers.

A computer model of the structures of each dendrimers **G1 – G6** was constructed using Spartan (Spartan Wavefunction, Inc., Irvine, CA, USA) with basic equilibrium geometry obtained by energy minimization. The cross sectional diameter were then obtained from an average of 10 determinations of the longest distances between two atoms.

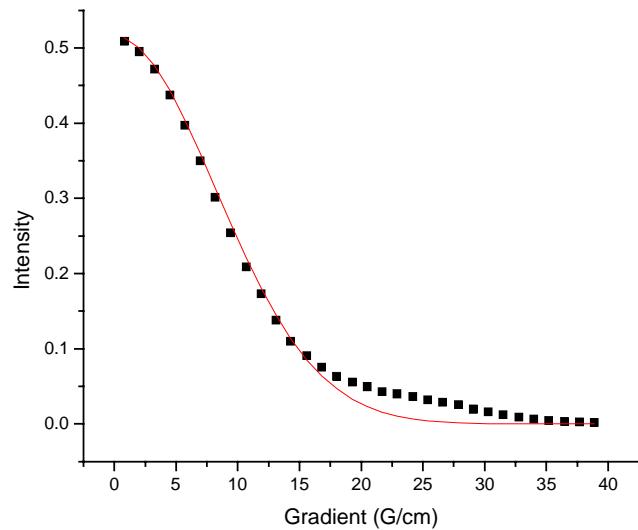


Figure S6 Fit of G1 self-diffusion data to the Stejskal-Tanner equation δ 1.8ms, Δ 50ms.

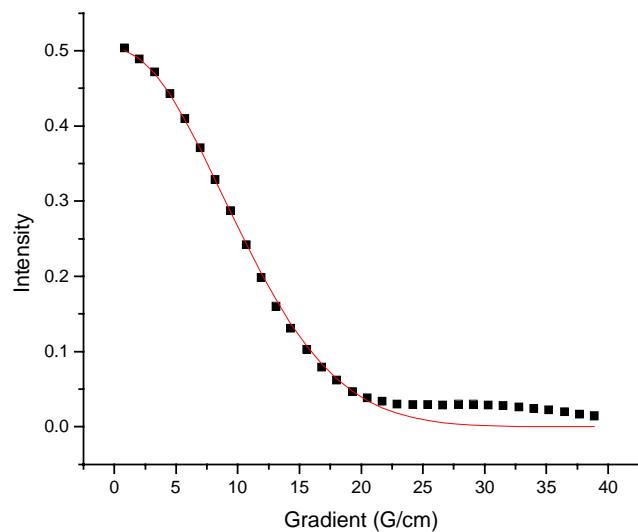


Figure S7 Fit of G2 self-diffusion data to the Stejskal-Tanner equation δ 1.6ms, Δ 50ms.

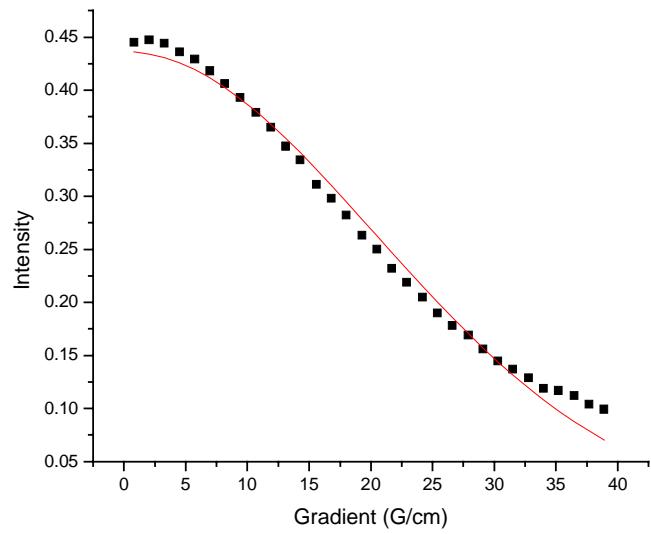


Figure S8 Fit of G3 self-diffusion data to the Stejskal-Tanner equation δ 1.4ms, Δ 50ms.

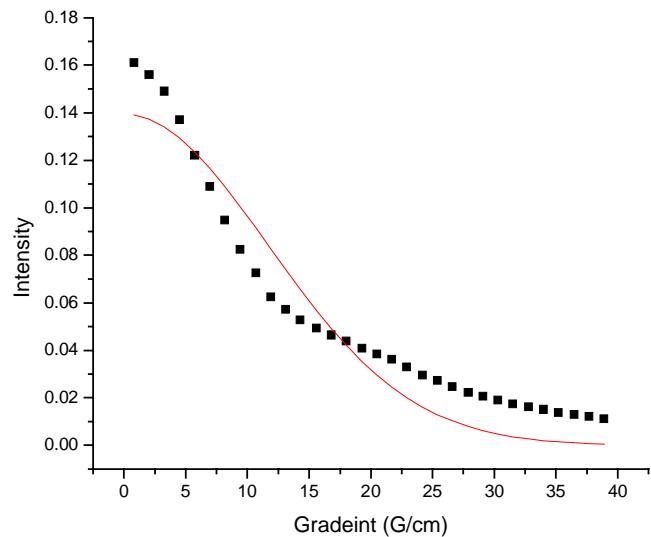


Figure S9 Fit of G4 self-diffusion data to the Stejskal-Tanner equation δ 2.4ms, Δ 100ms.

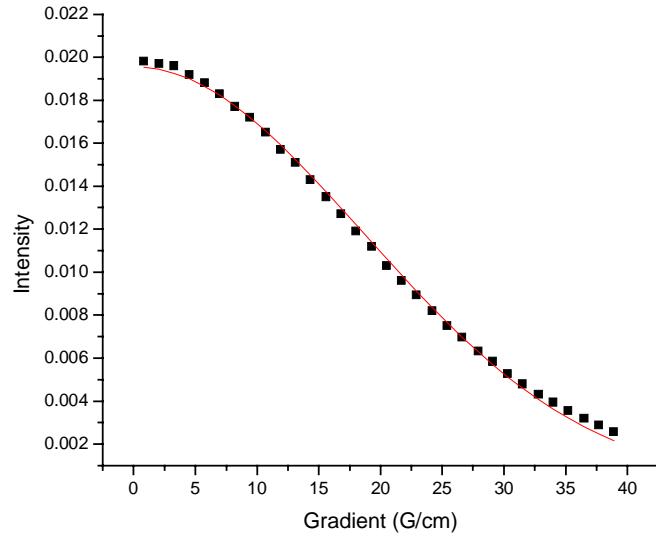


Figure S10 Fit of G5 self-diffusion data to the Stejskal-Tanner equation δ 2.4ms, Δ 100ms.

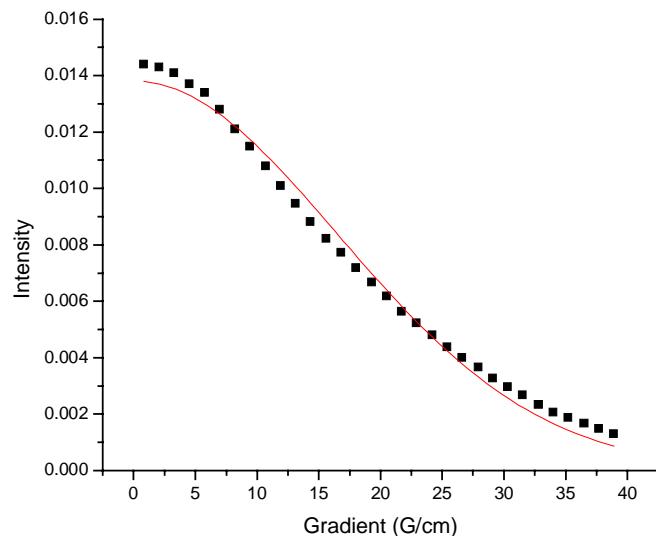


Figure S11 Fit of G6 self-diffusion data to the Stejskal-Tanner equation δ 2.6ms, Δ 100ms.