Subtle influence on alginate gel properties through host–guest interactions between covalently appended cyclodextrin and adamantane units

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Table S1. Yield stress values of alginate and functionalized alginate gels

System	σ* (Pa)
Alg	377
Alg-1,2-β-CD	913
Alg-1,3-β-CD	872
Alg-1,6-β-CD	2563
Alg-Ad	803
Alg-1,2-β-CD/Alg-Ad	3450
Alg-1,3-β-CD/Alg-Ad	6961
Alg-1,6-β-CD/Alg-Ad	9860

Table S2. Assignment of the main vibrational modes of unmodified alginate, functionalised alginates and mixtures of functionalized alginates

Xerogel	Wavenumber (cm^{-1}) [a]	Assignment [b]
Alg	3345, 3228 (s); broad 2934, 2853 (w) **1595** (s) **1425** (m) 1308 (w) 1144, 1113 (w) 1078 (sh), 1017 (s) *fingerprint region* 964, 938 (m) 887 (w) 820 (m)	ν(O-H), hydrogen bonded ν(C-H) $\nu_a(COO^-)$ $\nu_s(COO^-)$ δ(C-C-H) + δ(O-C-H) ν(C-O) + ν(C-C) + ν(C-O-C) ν(C-O) + ν(C-C) + δ(C-C-C) ν(C-O) + ν(C-C) + δ(C-C-O) (M+G) δ(C1-H) (M+G) δ(C-C-O) + δ(C-C-H) (M)
Alg-Ad	3348, 3230 (s); broad **1623** (sh, s) **1600** (s) **1433** (m) 1307 (w) 1146, 1114 (m) 1079, 1018 (m) *fingerprint region* 962, 940 (m) 888 (w) 821 (m)	ν(O-H) + ν(N-H), hydrogen bonded ν(C=O) $\nu_a(COO^-)$ $\nu_s(COO^-)$ + ν(C-N) + δ(N-H) δ(C-C-H) + δ(O-C-H) ν(C-O) + ν(C-C) + ν(C-O-C) ν(C-O) + ν(C-C) + δ(C-C-C) ν(C-O) + ν(C-C) + δ(C-C-O) (M+G) δ(C1-H) (M+G) δ(C-C-O) + δ(C-C-H) (M)
Alg-1,2-β-CD	3360, 3238 (s); broad **1623** (s) **1443** (w) 1150, 1113 (w) 1078, 1025 (m) *fingerprint region* 963, 941 (w) 823 (m)	ν(O-H) + ν(N-H), hydrogen bonded ν(C=O) ν(C-N) + δ(N-H) ν(C-O) + ν(C-C) + ν(C-O-C) ν(C-O) + ν(C-C) + δ(C-C-C) ν(C-O) + ν(C-C) + δ(C-C-O) (M+G) δ(C-C-O) + δ(C-C-H) (M)
Alg-1,2-β-CD/Alg-Ad	3350, 3230 (s); broad **1615** (s); less sharp, broader **1434** (m) 1149, 1115 (w) 1079, 1025 (m) *fingerprint region* 962, 940 (w) 890 (w) 820 (m)	ν(O-H) + ν(N-H), hydrogen bonded ν(C=O) ν(C-N) + δ(N-H) ν(C-O) + ν(C-C) + ν(C-O-C) ν(C-O) + ν(C-C) + δ(C-C-C) ν(C-O) + ν(C-C) + δ(C-C-O) (M+G) δ(C1-H) (M+G) δ(C-C-O) + δ(C-C-H) (M)

[a] s, strong; sh, shoulder; w, weak; m, medium; [b] ν, stretching; δ, deformation (bending)

Table S3. Rotational correlation time (τ) values for alginate samples in aqueous solution (1%)

System	$\tau \times 10^{10}$ (s)	$\tau \times 10^{10}$ (s) (mixture with Alg-Ad-T)
Alg-T	3.7	-
Alg-Ad-T	3.9	-
Alg-1,2-β-CD-T	7.3	6.6
Alg-1,3-β-CD-T	3.4	4.2
Alg-1,6-β-CD-T	3.9	4.2

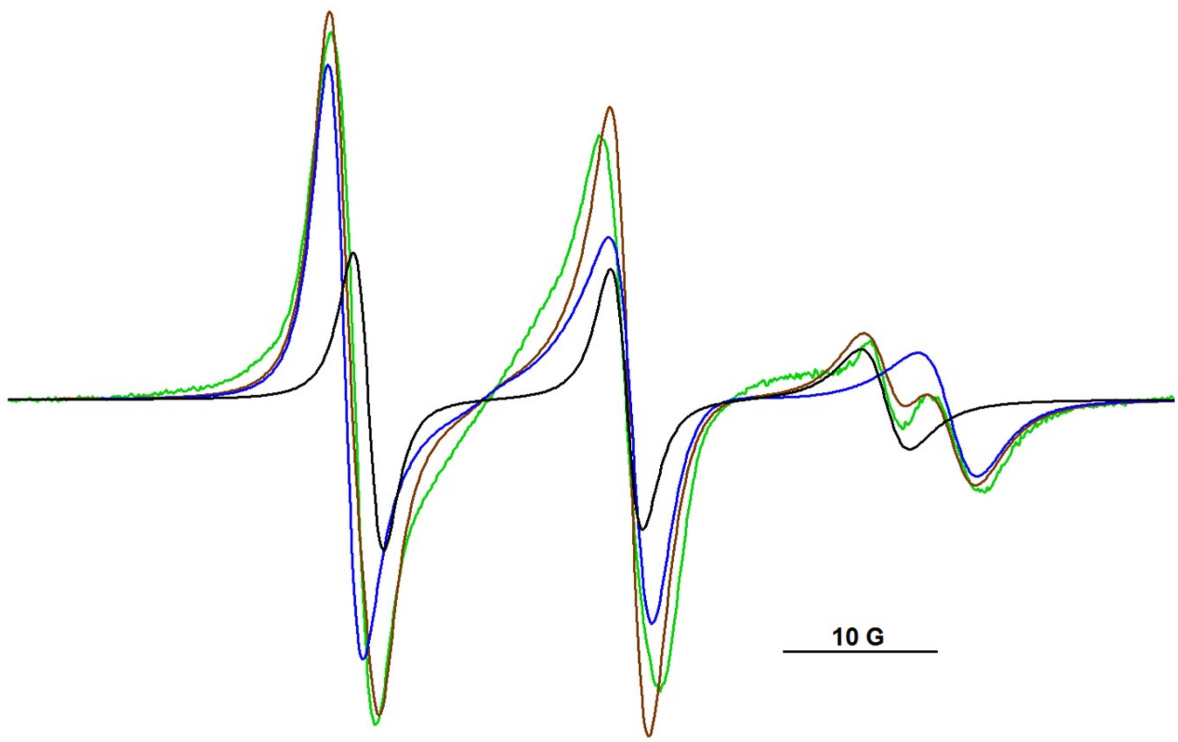

Fig. S1. The EPR spectra of 4-carboxy-TEMPO in Alg-1,2-β-CD gel: experimental (green), simulated (brown), slower component (blue), faster component (black).

Table S4. The ratio between the two components and the distance between outer peaks ($2A_{zz}$, in G) in the EPR spectra of spin-labelled alginate gels and their mixtures

System	**One alginate**		**Mixture of Alg-Ad-T and Alg-1,n-β-D-T**	
	Ratio slow component/fast component	$2A_{zz}$	Ratio slow component/fast component	$2A_{zz}$
Alg-Ad-T		57.4	-	-
Alg-1,2-β-CD-T	4.74	57.8	4.58	60.2
Alg-1,3-β-CD-T	3.66	62.1	4.64	63.5
Alg-1,6-β-CD-T	2.15	60.4	3.78	61.0

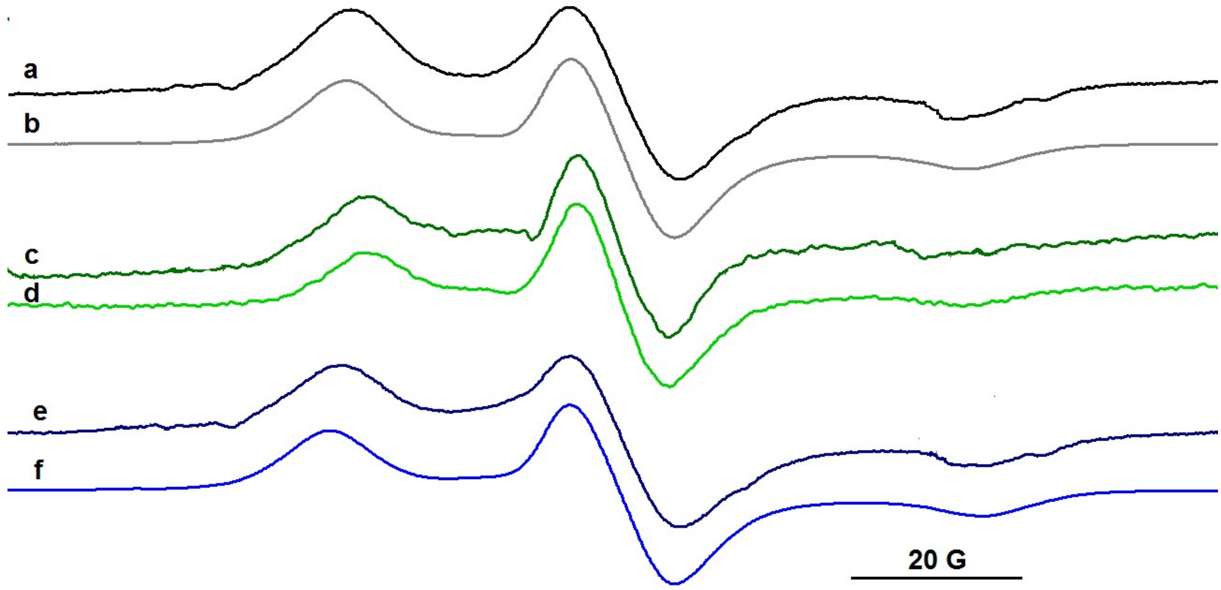

Fig. S2. The EPR spectra of alginates recorded at 120 K: a) Alg-1,2-β-CD-T solution, b) Alg-1,2-β-CD-T gel, c) 4-amino-TEMPO in Alg-1,2-β-CD solution, d) 4-amino-TEMPO in Alg-1,2-β-CD gel, e) Alg-1,2-β-CD-T solution in the presence of 1-adamantanecarboxylic acid, f) Alg-1,2-β-CD-T gel in the presence of 1-adamantanecarboxylic acid.