

Electronic supplementary information (ESI)

Figure S1. Dependence of the gel-sol phase transition, T_{gs} , on the gelator **1** concentration in benzene, toluene and *p*-xylene gels. The solid lines have no physical meaning and are included as a visual guide.

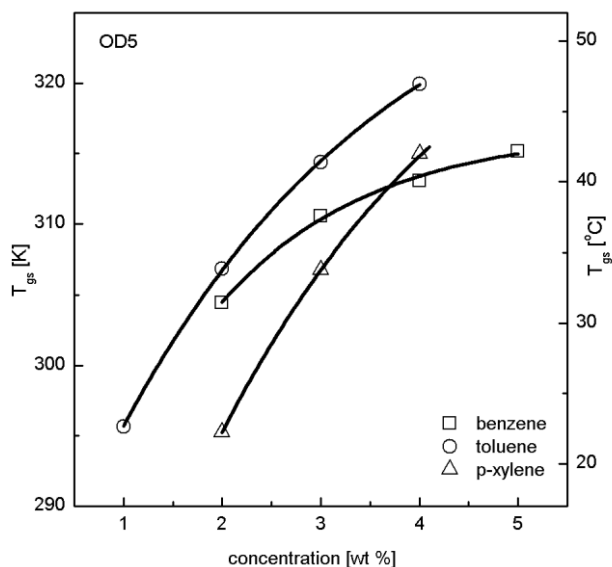


Figure S2. NMRD curves for non degassed bulk solvents measured as a function of the magnetic field strength reported as the proton Larmor frequency (bottom) and electron Larmor frequency (top). The solid lines are the best fit of eqn (7) to the experimental points.

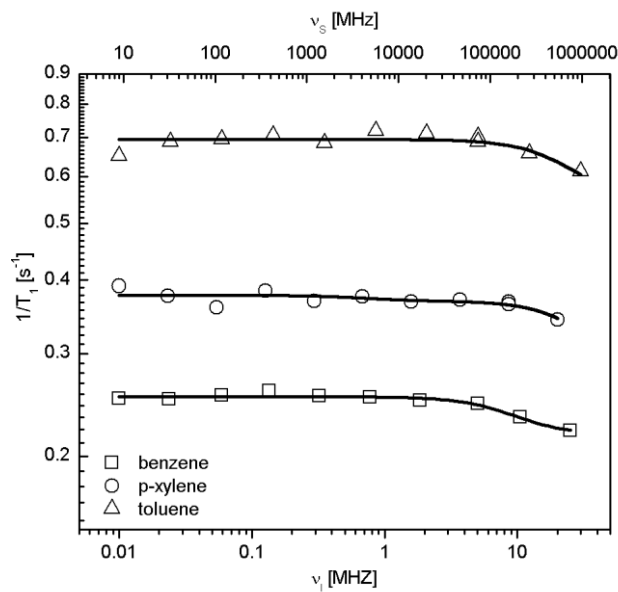


Table S1. Experimental and calculated vibrational transitions for gelator **1** molecule; ν - wavenumbers (cm^{-1}), I -IR intensity (km mol^{-1}), A – Raman scattering activity ($\text{\AA}^4 \text{amu}$).

Experiment ^(a)		Calculation ^(b)				Approximate description ^(d)
ν_{IR}	ν_{Raman}	ν	$\nu_{\text{nor}}^{(c)}$	I	A	
	156m	152	146	18.4369	8.0955	NH ₂ rck
	175w	164	158	5.4769	1.3468	def oop
	209vw	215	207	0.7117	5.7643	def ip
	245w	238	229	4.0521	2.3991	def oop
	279w	285	274	10.0547	1.7881	ring def oop
	318m	310	298	6.8261	7.2669	ring def oop
	334w	334	321	31.5746	2.2067	N-N-C b ip
	359w	359	345	4.1742	1.6383	benzene def oop
	376m	378	363	12.9336	6.3084	benzene def oop
426vw	426w	420	404	5.3618	5.724	benzene def oop
466vw	462w	484	465	3.0401	5.3972	ring def ip
488vw	487vw	514	494	116.4822	6.5129	N-H b oop
519vw	522w	564	542	13.4105	6.9406	C-C-C b oop
	567w	617	593	2.0383	6.0833	C-C-N b ip
646w	650s	656	631	20.6637	14.7442	C-C-C b ip
677vw	681w	681	655	10.4994	2.8726	C-C-C b oop
713vw	714vw	733	705	10.0646	3.6574	C-C-C b oop
756w	753s	770	740	13.5028	7.0123	C-N b oop+C-H b oop
769sh	769w	774	744	9.9448	4.9048	C-N b oop+C-H b oop
833w		852	819	1.6359	2.044	C-O str+CH ₂ rck
846w	851m	860	827	20.7645	11.8539	NO ₂ scis+N-N-N b ip
859vw	862m	872	838	5.6494	10.8539	CH ₂ rck
917w	920w	952	915	16.1423	7.1553	C-C-C b ip+NH ₂ wag
942w	943w	972	934	90.6577	11.413	C-H b oop+CH ₂ rck
977w	980vw	1029	989	3.7884	10.325	C-N str
	1016vw	1060	1019	34.1106	18.4477	C-N-C b ip
1044w	1045w	1084	1042	12.9285	2.4798	CH ₂ rck
1067w	1068vw	1098	1056	22.2418	4.8487	C-N str
1081vw	1080w	1106	1063	2.3469	6.8098	C-N str+NH ₂ wag
1113m	1112w	1131	1087	90.8016	13.079	C-O str+C-C str
1118sh	1122vw	1168	1123	20.8797	7.7378	C-N str+C-H b ip
1150vw	1150vw	1196	1150	54.4868	20.0334	C-N str+C-H b ip
1176vw	1178sh	1216	1169	11.9833	73.1072	N-N str+C-C str
1191w	1191m	1238	1190	18.2149	16.6461	CH ₂ tw
1215w	1218m	1260	1211	171.0506	26.8502	C-N str+CH ₂ tw
1236m	1241m	1281	1231	50.7907	5.9455	C-H b ip+CH ₂ tw
1257w	1261w	1302	1252	228.5949	139.6885	C-C str+N-N str+C-H b ip
1276w	1281s	1314	1263	28.9892	39.1447	C-C str+C-H b ip
1293w	1290sh	1327	1276	57.652	24.3401	CH ₂ tw
1302w	1299s	1333	1281	33.8362	24.4048	CH ₂ tw
1333m		1351	1299	8.0097	6.8558	NH ₂ tw
1345m	1348vs	1361	1308	205.3756	108.2845	C-N str
1353sh		1413	1358	93.8967	4.1007	C-N str+CH ₂ wag
1380w	1375sh	1436	1380	21.9244	28.5344	C=C str+C-N str
1450w	1449vw	1490	1432	187.7616	29.9071	N-H b ip+CH ₂ scis
1457sh	1464vw	1502	1444	94.2035	4.4488	N-H b ip+CH ₂ scis
1496m	1496vw	1539	1479	29.2301	31.0322	C-N str
1521vs	1521vw	1566	1505	69.9167	76.6854	C=C str+N=O asym str
1555sh	1555m	1584	1523	210.2549	21.457	C=C str+N=O asym str
1616vs	1619m	1652	1588	323.6646	264.2258	C=C str
1636m		1705	1639	122.068	3.9605	NH ₂ scis+C=O str
1657m	1650m	1724	1657	191.4801	170.8803	C=O str+NH ₂ scis
2832vw		2961	2846	45.8613	137.7087	CH ₂ sym str
2860w	2863vw	2972	2857	61.2436	235.341	CH ₂ sym str
2898vw	2896vw	2992	2876	48.4888	65.512	CH ₂ sym str
2923vw	2924vw	3017	2900	36.0166	68.4949	CH ₂ sym str
2963vw	2968vw	3093	2973	13.3159	45.4619	CH ₂ asym str
	3043vw	3157	3035	6.9933	29.2384	CH ₂ asym str
3077vw	3080vw	3196	3072	0.1211	52.6515	C-H str in benzene
3102vw	3100vw	3215	3091	5.4163	115.6617	C-H str in benzene
3310m	3311vw	3461	3327	2.2865	197.7792	NH ₂ sym str
3343m	3340vw	3527	3391	8.5385	75.331	NH ₂ asym str
3480sh		3621	3481	43.4442	41.3151	N-H str

^(a) vs=very strong, s=strong, m=medium, w=weak, vw=very weak, sh=shoulder.

^(b) Calculations have been performed for OD5 at BLYP/6-311++G(d,p) theory level.

^(c) Calculated frequencies were scaled by the factor of 0.9613 [Wong1996].

^(d) Approximate mode description: str=stretching, def=deformation, b=bending, wag=wagging, tw=twisting, rck=rocking, scis=scissoring, ip=in-plane, oop=out of plane, sym=symmetrical, asym=antisymmetrical.

Table S2. Excitation energies (ΔE in eV), wavelength (λ in nm), oscillator strengths f , and characterization of the excited singlet states for the gelator molecule.

Experiment		Theory ^(a)			Charakter ^(b)
ΔE	λ	ΔE	λ	f	
3.12	398	3.02	411	0.0411	HOMO→LUMO (91%) $\pi \rightarrow \pi^*$
4.28	290	4.28	290	0.1914	H-7→LUMO (10%), H-3→LUMO (30%), HOMO→L+1 (46%)
		4.75	261	0.1328	H-7→LUMO (21%), H-6→LUMO (15%), H-4→LUMO (26%) $\pi \rightarrow \pi^* + n \rightarrow \pi^*$
5.17	240	5.17	240	0.0476	H-10→LUMO (20%), H-9→LUMO (20%), H-7→LUMO (26%), H-6→LUMO (12%) $\pi \rightarrow \pi^* + n \rightarrow \pi^*$

(a)TD-B3LYP/6-311++G(d,p) method has been employed to obtain the energies of the first 150 singlet-singlet electronic transitions

(b)H means the highest occupied molecular orbital (HOMO), L means the lowest unoccupied molecular orbital (LUMO)