Supporting Information

Donor-Acceptor Interaction Promoted Gelation: Visual Observation of Color Change

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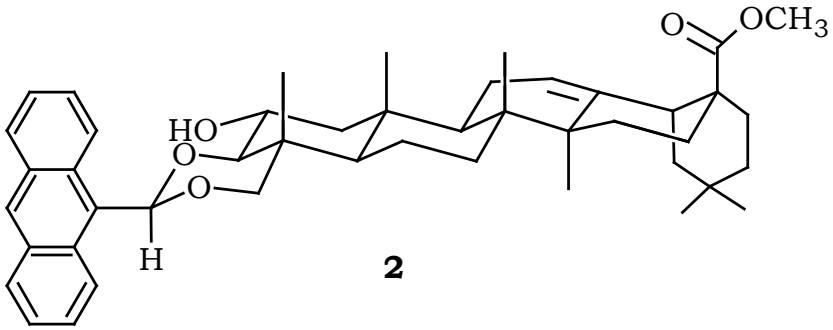

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Anthryilidine methyl arjunolate 2: A solution of methyl arjunolate[1] (1 g, 1.99 mmol) in dry benzene (6 mL) was treated with anthracene-9-aldehyde (0.492 g, 2.34 mmol), perchloric acid (0.04 mL, 70% solution) and the mixture was stirred at room temperature over molecular sieves (4Å) for 5h. The crude product was diluted with chloroform (100 mL) and washed with 5% sodium bicarbonate (3X 20 mL), brine (3X 20 mL) and dried over anhydrous sodium sulphate. Volatiles were removed under reduced pressure and the crude product was purified by column chromatography (Si-gel, 100-200 mesh) using 5% ethyl acetate/ chloroform to afford a foamy solid (1.17 g) in 85% yield.

R_f = 0.36 (70% chloroform/ petroleum ether)

MP = 230 ˚C

^{1}H NMR (600 MH$_z$, DMSO-d$_6$) δ: 8.88 (d, J = 9.0 Hz, 2H), 8.66 (s, 1H), 8.09 (d, J = 7.8 Hz, 2H), 7.55-7.50 (m, 4H), 6.95 (s, 1H), 5.22 (app. s, 1H, 12-H), 4.55 (s, 1H, -O-H), 3.95 (d, J = 10.8, 1H, 23-H$_a$), 3.84 (d, J = 10.8 Hz, 1H, 23-H$_b$), 3.80 (br. s, 1H, 2-H), 3.65 (d, J = 10.2 Hz, 1H, 3-H), 3.55 (s, 3H), 2.79 (app. d, J = 13.2 Hz, 1H), 2.10 - 0.68 (terpenoid protons, 20H), 1.42 (S, 3H), 1.16 (S, 3H), 1.05 (S, 3H), 0.90 (S, 3H), 0.89 (s, 3H), 0.69 (s, 3H).

(1) Bag, B.G.; Pramanik, S.R.; Maity, G.C. *Supramol. Chem.* **2005**, 297.

^{13}C NMR (150 MHz, $CDCl_3$) δ: 177.27, 143.60, 131.01, 129.40, 129.18, 128.81, 128.50, 125.95, 125.46, 125.10, 121.71, 101.45, 91.68, 79.06, 63.57, 51.57, 50.76, 48.68, 47.20, 46.12, 45.47, 41.37, 40.99, 38.96, 37.81, 37.19, 33.22, 32.84, 32.06, 31.81, 30.46, 27.19, 25.78, 23.44, 22.93, 22.64, 17.35, 17.16, 16.58, 15.85

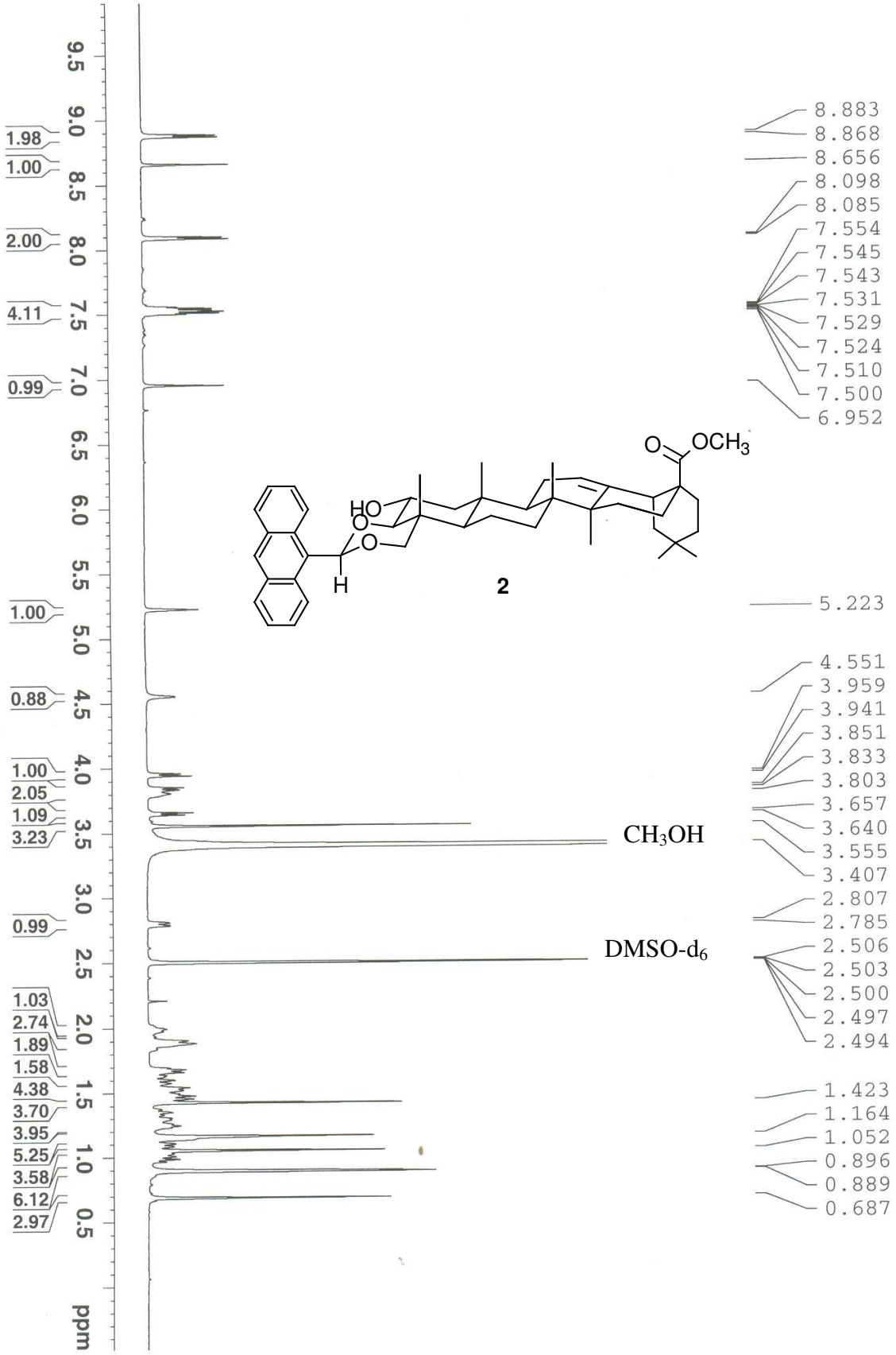
FT-IR: ν_{max} (neat, cm^{-1}) 3583, 3501, 3087, 3051, 2947, 2863, 1723, 1658, 1624, 1560, 1525, 1456, 1433, 1391, 1160, 1109, 1050.

$[\alpha]_D^{298}$ = + 28.51 (c 0.206, $CHCl_3$)

λ_{max} (MeOH, log ε) = 254.0 (4.46), 346.0 (3.73), 364.0 (3.90), 384.0 (3.86).

HRMS (ESI): *m/z* calcd ($C_{46}H_{58}O_5Na$) 713.4182, found 713.4219 ($M + Na^+$).

[1]H-NMR of Compound **2** (600 MHz) in DMSO-d_6



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^{13}C-NMR of compound **2** (150 MHz) in DMSO-d_6

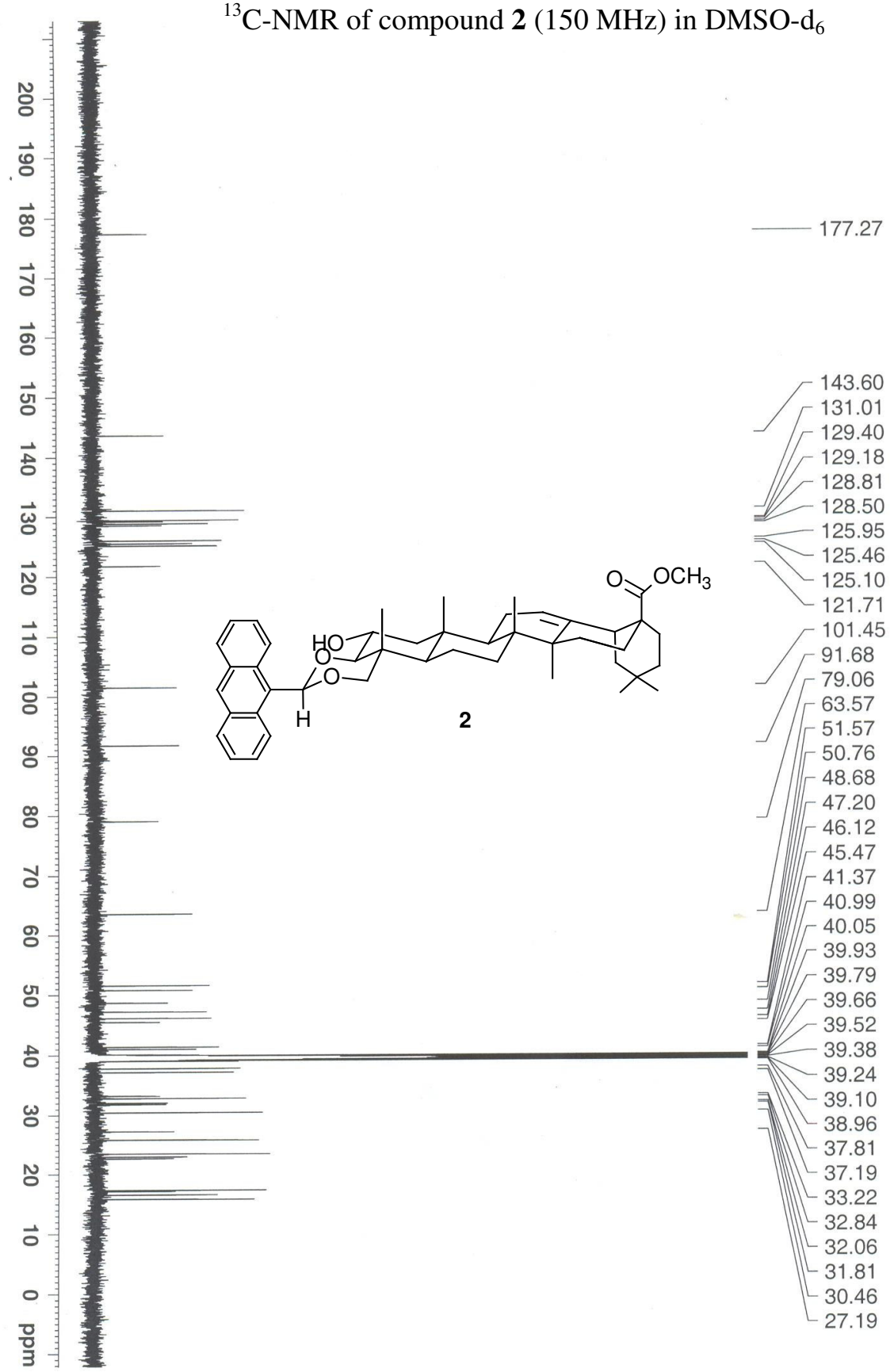

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Table 1 : Gelation Test Results of 1:1 mixture of compound 2 and picric acid

Entry	**Solvent**	**Conc. (g/100 mL)**	**State**	**Tgel (ºC)**
1	Methanol	3.4	P	-
2	Ethanol	2.5	G	39
3	n-propanol	6.4	G	38
4	2-Propanol	2.0	G	36
5	n-butanol	2.0	G	42
6	2-Butanol	2.0	G	29
7	^{t}Butanol	1.43	P	-
8	Cyclohexanol	5	G	42
9	n-octanol	5	G	35
10	Diethylene glycol	10	G	48
11	Petroleum ether	1.0	I	-
12	DMF	6.4	S	-
13	Benzene	6.4	S	-
14	CH_2Cl_2	3.2	S	-
15	$CHCl_3$	6.4	WG	-
16	CCl_4	0.45	G	35
17	$CHCl_3$ / CCl_4 (1:20)	4.76	G	51
18	P.E./$CHCl_3$ (6:1)	1.42	G	41

Table 2: Gelation Test Results of 1:1 mixture of compound 2 and methyl 3,5 dinitro benzoate

Entry	Solvents	Conc (g/100mL)	State	T_{gel} (°C)
1	MeOH	0.71	P	-
2	EtOH	0.8	FG	-
3	n-Propanol	0.8	FG	-
4	2-Propanol	0.625	G	55
5	2-Butanol	1.0	G	58
6	Cyclohexanol	0.625	G	32
7	Diethylene glycol	2.66	P	-
8	Diethyl ether	1.6	S	-
9	$CHCl_3$	3.2	S	-
10	$CHCl_3$/2-Propanol	0.94	FG	-
11	$CHCl_3$/2-butanol	2.9	FG	-
12	CCl_4	1.6	P	-
13	Benzene	2.66	S	-
14	Toluene	2.66	S	-
15	n-Butanol	1.25	G	56
16	^{t}Butanol	0.357	P	-
17	n-Octanol	2.5	G	69
18	$CHCl_3$/ Pet. Ether (1:6)	1.64	P	-
19	$CHCl_3$/ CCl_4(1:20)	0.79	S	-
20	CH_2Cl_2	2.5	S	-
21	DMF	2.5	S	-

Table 3: T_{gel} of compound 2 and picric acid at various molar ratios in carbon tetrachloride

Sl. No.	Molar ratio of compound **2** & picric acid	T_{gel} (^{o}C)
1	1: 0.508	41
2	1:0.8475	46
3	1:1.01	49
4	1:1.1866	45
5	1:1.406	41

Plot of T_{gel} vs different molar ratio of compound 4 and 2

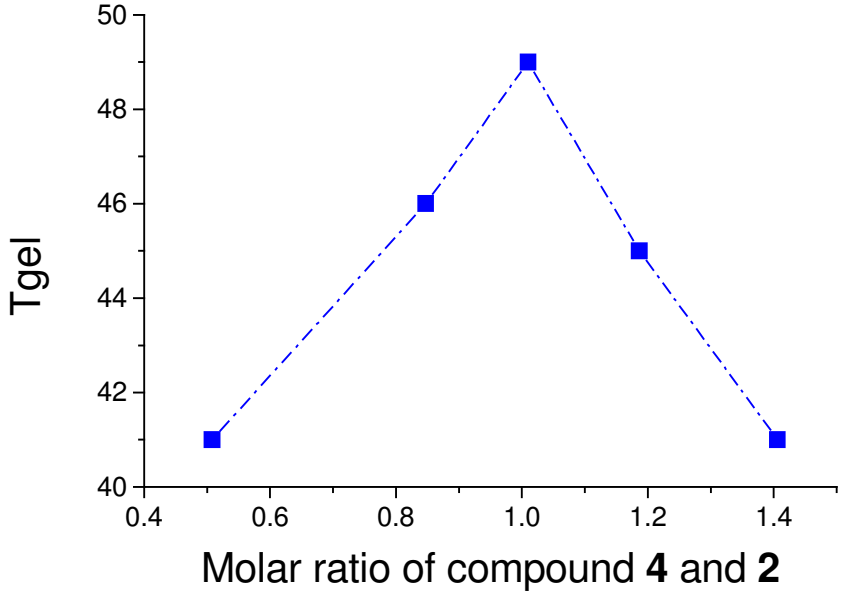


Table 4 : Gelation Test Results of 1:1 mixture of compound 3 and picric acid

Entry	Solvents	Conc (g/100mL)	State
1	Methanol	2.5	S
2	Ethanol	5.0	S
3	n-propanol	5.0	S
4	2-Propanol	5.0	S
5	n-Butanol	1.25	S
6	2-Butanol	5.0	S
7	Cyclohexanol	5.0	S
8	^{t}Butanol	2.5	S
9	n-Octanol	5.0	S
10	CCl_4	1.66	C
11	Benzene	5.0	S
12	Toluene	5.0	S
13	$CHCl_3$	3.33	S
14	CH_2Cl_2	5.0	S
15	Ethyl acetate	3.33	S
17	Diethylene glycol	5.0	S
18	Triethylene glycol	5.0	S
19	DMF	5.0	S
20	Pet. ether	5.0	I

C = Crystal, P = Precipitate, I = Insoluble, S = Soluble.

Table 5: Gelation Test Results of 1:1 mixture of compound 3 and methyl 3,5 dinitrobenzoate in 1:1 molar ratio

Entry	Solvents	Conc (g/100mL)	State
1	Methanol	2.86	C
2	Ethanol	10	C
3	n-propanol	10	C
4	2-Propanol	10	C
5	n-Butanol	10	C
6	2-Butanol	10	C
7	Cyclohexanol	10	C
8	^{t}Butanol	10	P
9	n-Octanol	10	S
10	CCl_4	10	S
11	Benzene	10	S
12	Toluene	10	S
13	$CHCl_3$	20	S
14	CH_2Cl_2	20	S
15	Ethyl acetate	3.33	S
17	Diethylene glycol	10	P
18	Triethylene glycol	10	P
19	DMF	20	S
20	Pet. ether	2.0	I

C = Crystal, P = Precipitate, I = Insoluble, S = Soluble.

Table 6: Gelation Test Results of 1:1 mixture of compound 6 and picric acid

Entry	Solvents	Conc (g/100mL)	State
1	Methanol	5	S
2	Ethanol	5	C
3	n-propanol	2.5	C
4	2-Propanol	2.5	P
5	n-butanol	5	C
6	2-Butanol	3.33	C
7	Cyclohexanol	2.5	C
8	n-octanol	2.5	C
9	Diethylene glycol	5	S
10	Petroleum ether + $CHCl_3$ (4:3)	3.3	C
11	CCl_4	2.5	C
12	Benzene	5	S
13	Toluene	5	S
14	$CHCl_3$	2.5	S

Thermodynamic Parameters[2]

The thermoreversible melting of a two coomponent gel can be expressed as:

Gel $\rightleftharpoons$ liquid

For a two comoponent gel containing equimolar concentration of gelator (anthrylidene derivative **2**) and guest, the equilibrium constant can be expressed as:

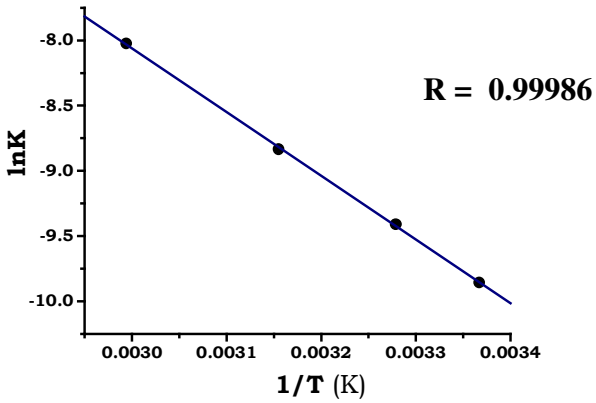
K = [Guest].[Gelator]/[Gel]

Assuming unit activity of the gel and taking concentration of the solution to be be equal to the dissolved concentration of the gelator (anthrylidene derivative **2**) and the guest, the equilibrium constant can be expressed as: K = [Guest].[Gelator].

The Gibbs free energy change during gel melting can be expressed as:

$\Delta G^o = - RT\ln K = \Delta H^o - T\Delta S^o$, Hence, $\ln K = - \Delta H^o/R .(1/T) + \Delta S^o/R$

The gel melting temperature (T_{gel}) increases with increasing concentration of the "solutes". A plot of lnK vs 1/T allowed us to calculate the thermodynamic parameters. A representative plot for a gel in cyclohexanol having anthrylidene derivative **2** and methyl 3,5-dinitrobenzoate in (1:1) ratio is given in figure below:



(2) Rizkov, D.; Gun, J.; Lev, O.; Sicsic, R.; Melman, A. *Langmuir* **2005**, *21,* 12130.

From the slope we obtain - $\Delta H^o/R$ = - 4888.32121 and from the intercept we obtain $\Delta S^o/R$ = 6.60502

The thermodynamic parameters are: ΔS^o = 54.9 J/mol/ºK, ΔH^o = 40.6 kJ/mol and ΔG^o = 24.3 kJ/mol.