Electronic Supplementary Material (ESI) for Soft Matter.

THERMODYNAMICS, MORPHOLOGY AND MOLECULAR STRUCTURE OF MOLECULAR COMPOUNDS IN TRISAMIDE TRIARYLAMINE ORGANOGELS AND PSEUDO-ORGANOGELS

Ganesh VISWANATHA-PILLAI, Andreas VARGAS-JENTZSCH, Alain CARVALHO, Guillaume FLEITH, Odile GAVAT, Emilie MOULIN, Nicolas GIUSEPPONE and Jean-Michel GUENET *

Institut Charles Sadron
CNRS-Université de Strasbourg
23 rue du Loess, BP84047
67034 STRASBOURG, Cedex2, France

Supplementary information

structureII	$q_{strucII}$	$d_{strucII}$	*hk*	Int	q_{tolu}	d_{tolu}	d_{calc}	Lattice toluene C_1
a = 3.47(5) nm b = 5.03(9) nm γ = 90° A = 17.51 nm^2	2.193	2.864	*11*	VS	1.97	3.189	3.2	a = 3.66(5) nm b = 6.5 nm γ = 90° A = 24.16 nm^2
	3.619	1.736	*20*	S	3.43	1.831	1.831	
	4.388	1.432	*22*	S	3.95	1.59	1.6	
			06	VW	5.589	1.12	1.08	
	6.588	0.954	*33*	VW	5.89	1.066	1.066	

Table S1: *Experimental and calculated scattering vectors and spacings $q_{strucII}$, $d_{strucII}$, from peak position of the structure II observed in the solid state[S1], and of compound C_1 in toluene, q_{tolu}, d_{tolu}, d_{cal}. Signal intensity code: VS = very strong, S = strong, M = medium, W = weak, VW = very weak; (hk) are the Miller indices of the reflections, for this structure h+k= 2n; a, b, γ, A: lattice parameters and lattice area.*

hk	Int	q_{tolu}	d_{tolu}	d_{calc}	Lattice toluene C_2 et C_3
11	VS	1.779	3.53	3.53	a = 3.72 nm b = 11.22 nm γ = 90° A = 41.74 nm^2
20	S	3.375	1.86	1.86	
22	S	3.547	1.771	1.765	
17?	W	4.56	1.378	1.46	
33	W	5.31	1.183	1.176	
28	VW	5.769	1.089	1.11	
44	VW	7.085	0.887	0.8825	

Table S2: *Experimental scattering vectors and spacings q_{tolu}, d_{tolu},from the peak position of compound C_2 in toluene and calculated spacings d_{cal} from the proposed 2-D lattice. Signal intensity code: VS = very strong, S = strong, M = medium, W = weak, VW = very weak; (hk) are the Miller indices of the reflections; a, b, γ, A: lattice parameters and lattice area.*

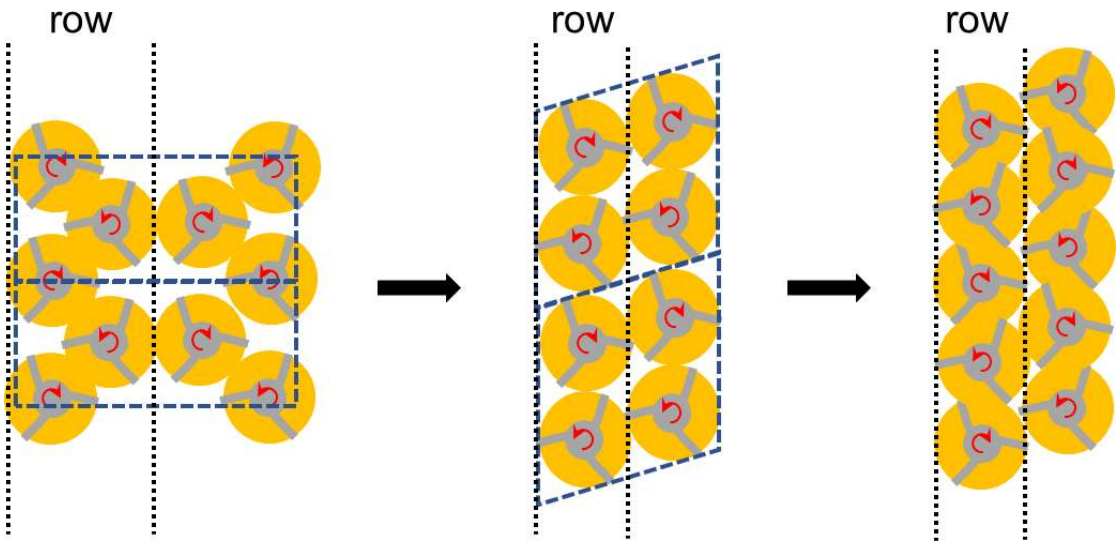

Figure S1: *Schematic break down of the way TATA molecular compounds are liable to produce rows containing regularly-alternating right and left-handed helices. By shrinking the row the rhombohedral structure can be produced, where right and left helices alternate. This in turns gives adjacent, decorrelated rows, which entails the observation of only one diffraction peak arising from the intermolecular correlation within the rows.*

$$\begin{array}{cccccc} d_{11} & d_{21} & d_{31} & d_{41} & d_{51} & d_{61} \\ d_{12} & d_{22} & d_{32} & d_{42} & d_{52} & d_{62} \\ d_{13} & d_{23} & d_{33} & d_{43} & d_{53} & d_{66} \\ d_{14} & d_{24} & d_{34} & d_{44} & d_{54} & d_{64} \\ d_{15} & d_{25} & d_{35} & d_{45} & d_{55} & d_{65} \\ d_{16} & d_{26} & d_{33} & d_{46} & d_{56} & d_{66} \end{array}$$

Figure S2: *Matrix for different spacing between cylinders d_{ij} in the intermolecular terms S(q) in the case of six cylinders arranged in a row (for details see text). The colours define diagonals corresponding to cylinders spaced apart by the same distance.*

The intermolecular term for correlated cylinders is given by[S2]:

$$S(q) = \frac{1}{N^2}\left[\sum_{i=1}^{N}\sum_{j=1}^{N} J_o\left(q d_{ij}\right)\right] \quad (1)$$

Where N is the number of cylinders.

The matrix shown in figure S1 illustrates the double sum of relation S1 when cylinders are arranged in a row. As is apparent, the d_{ij} in diagonals have the same value. By introducing *kd*, where k is an integer varying from 1 to N-1, and *d* the distance between two adjacent cylinders, equation S1 can be simply rewritten as a single sum through:

$$S(q) = \frac{1}{N^2}\left[N + \sum_{k=1}^{N-1} 2(N-k) J_o(qkd)\right] \quad 2$$

The 2(N-k) coefficients can be easily calculated for use in software such as Origin (see figure S3).

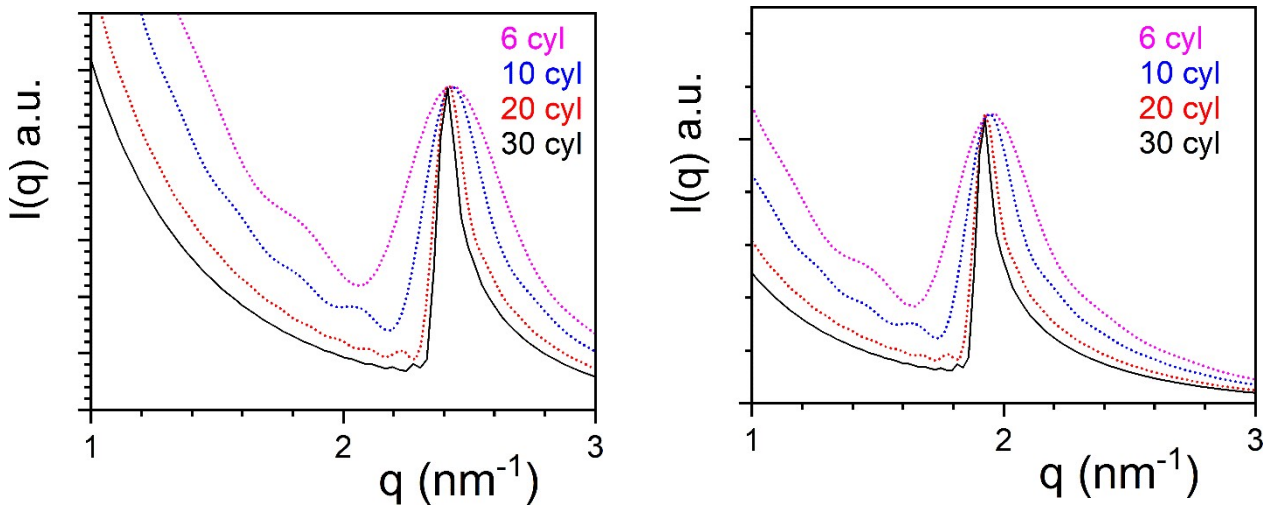

Figure S3: *Evolution of the diffracted intensities for cylinders arranged in a row calculated from relation (2). As can be seen the peak narrows with increasing the number of cylinders with estimated FWHM of 0.39, 0.28, 0.13 and 0.1.* ***left****) d= 2.63 nm;* ***right****) d= 3.3 nm*

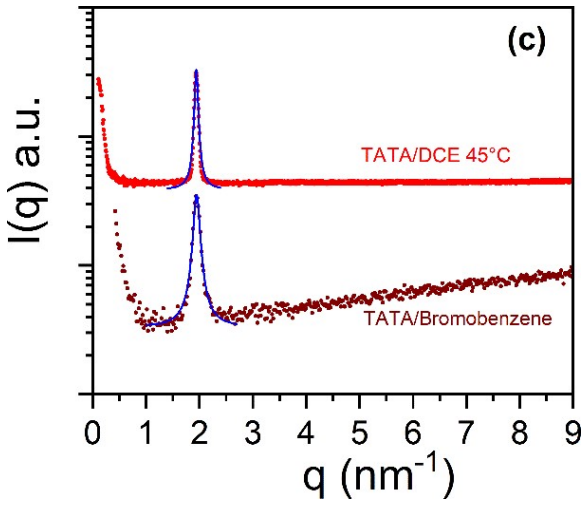

Figure S4: *comparison of the diffraction patterns of TATA/DCE at T= 45°C (red) and TATA/bromobenzene (brown), the latter from previous results*[S3]*. blue lines= fits with Lorentz functions.*

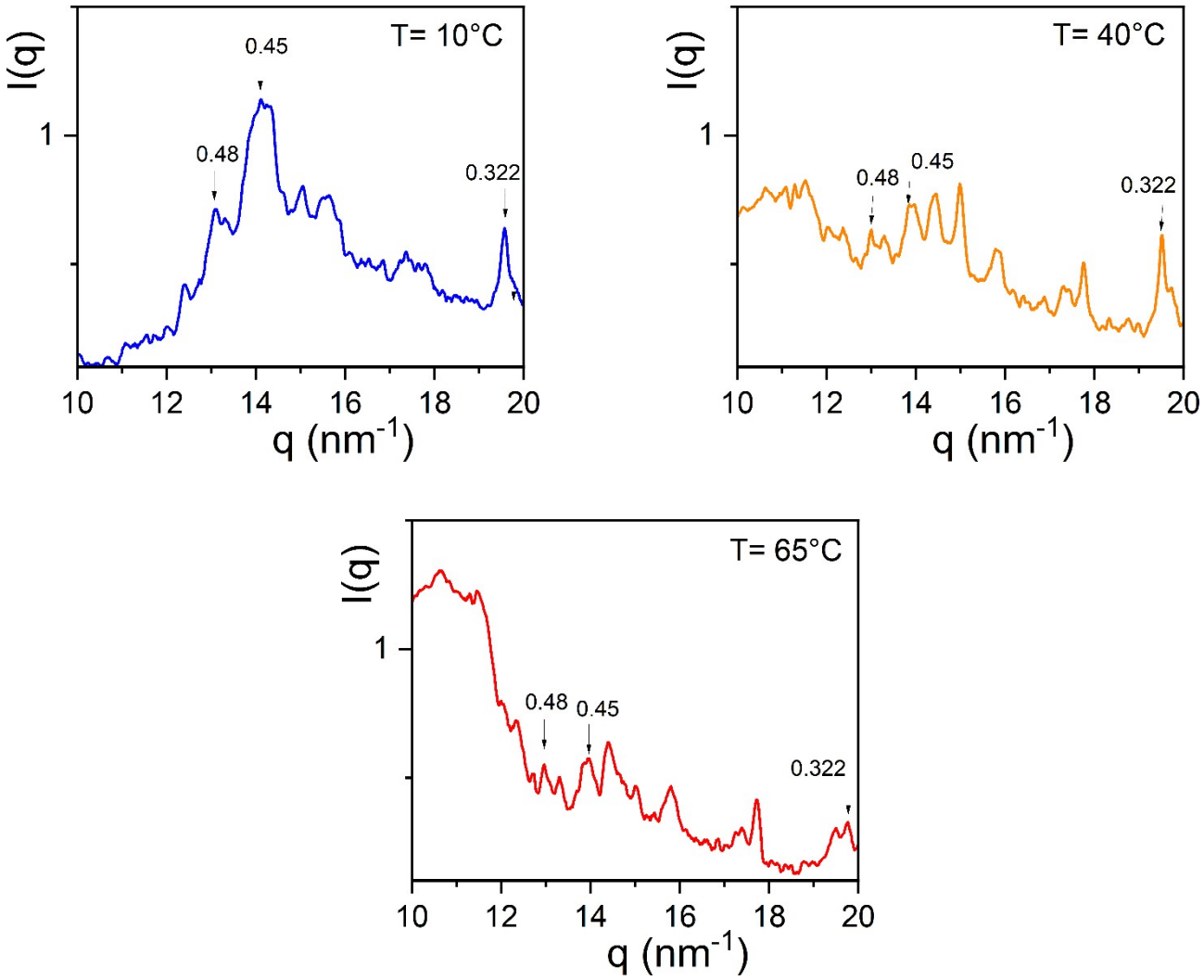

Figure S6: *Wide angle X-ray scattering for TATA-Toluene at different temperatures (as indicated). The reflections at d= 0.48 nm, 0.45 nm and 0.32 nm are typical from the TATA molecules piling[S4]. The distance 0.48 nm is associated with the N-N spacing of adjacent TATA molecules.*

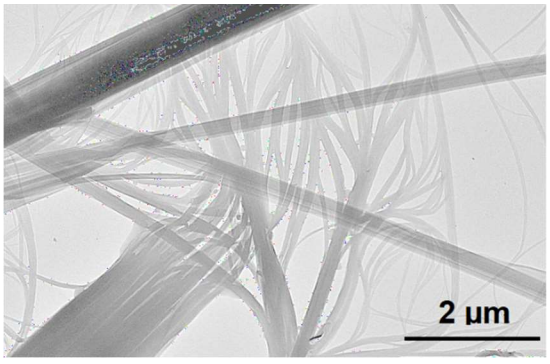

Figure S6: *Observation by transmission electron microscopy from dilute systems in TCE. This picture highlights the peeling of the TATA larger fibrils thus forming smaller curved fibrils. The fraying allows random connections between fibrils, which gives a physically-cross-linked network.*

REFERENCES

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