# Supplementary information 

EVIDENCE BY NEUTRON DIFFRACTION OF MOLECULAR<br>COMPOUNDS IN TRIARYLAMINE TRIS-AMIDE ORGANOGELS AND IN<br>THEIR HYBRID THERMOREVERSIBLE GELS WITH PVC.<br>GUENET $^{1 *}$, Jean-Michel ; DEMÉ ${ }^{2}$; Bruno; GAVAT ${ }^{1}$; Odile; MOULIN ${ }^{1}$; Emilie; GIUSEPPONE ${ }^{1}$, Nicolas<br>1 Institut Charles Sadron<br>CNRS-Université de Strasbourg<br>23 rue du Loess, BP84047<br>67034 STRASBOURG, Cedex2, France<br>2 Institut Laue-Langevin<br>71 avenue des Martyrs CS 20156<br>38042 GRENOBLE Cedex 9 - France

| component | TATA | BrBzH | BrBzD | o-DCBH | o-DCBD | TCEH | TCED | PVC |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $A=\sum b_{i} \times 10^{12} \mathrm{~cm}$ | 8 | 2.8 | 8.03 | 4.4 | 8.59 | 4.41 | 6.51 | 1.17 |
| $\frac{A}{v_{m}}$ | 0.011 | 0.0264 | 0.076 | 0.039 | 0.077 | 0.042 | 0.062 | 0.030 |
| $\frac{Z_{e}}{v_{m}}$ | 0.583 | 0.72 | 0.72 | 0.68 | 0.68 | 0.78 | 0.78 | 0.71 |

Table S1: Scattering amplitudes ${ }^{18}$ of the different components used in the present study obtained by summing the scattering length $b_{i}$ of the constituting atoms, together with the amplitude per unit molar volume $\left(v_{\mathrm{m}}\right)$, and the number of electrons $Z_{\mathrm{e}}$ per unit molar volume. The latter allow comparison between the different radiations and components.


Figure S1: theoretical curves for hexagonal packing and for arrangement in a row calculated from relation 4 . The number of helices is indicated.

| $\mathrm{q}_{\text {BrBZH }}$ | $\mathrm{d}_{\text {BrBZH }}$ | $\mathrm{q}_{\text {BrBZD }}$ | $\mathrm{d}_{\text {BrBZD }}$ | $\mathrm{q}_{\text {oDCBH }}$ | $\mathrm{d}_{\text {oDCBH }}$ | $\mathrm{q}_{\text {oDCBD }}$ | $\mathrm{d}_{\text {oDCBD }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1.96 | 3.2 | 1.96 | 3.2 | 2.005 | 3.134 | 2.005 | 3.134 |
|  |  | 3.469 | 1.81 | 3.38 | 1.859 | 3.366 | 1.867 |
|  |  | 5.76 | 1.091 | 5.48 | 1.146 | 5.483 | 1.146 |

Table S2: Diffraction peaks position $\mathrm{q}\left(\mathrm{nm}^{-1}\right)$ in TATA/BrBZ and TATA/o-DCB at T $=20^{\circ} \mathrm{C}$, and the corresponding distances (nm) calculated by means of Bragg's law. Values in red italics indicate very week peak.

| $\mathrm{q}_{\exp }$ <br> $\left(\mathrm{nm}^{-1}\right)$ | $\mathrm{d}_{\exp }$ <br> $(\mathrm{nm})$ | $\mathrm{I}(\mathrm{q})$ | $h k$ | FWHM | $\mathrm{d}_{\text {cal }}$ <br> $(\mathrm{nm})$ | Lattice parameters <br> TATA/TCE | Lattice parameters <br> structure $\mathrm{I}^{13}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 2.22 | 2.86 | S | 11 | 0.17 | 2.86 |  |  |
| 2.5 | 2.51 | S | 04 | 0.13 | 2.51 |  |  |
| 2.94 | 2.14 | VS | 13 | 0.15 | 2.22 | Orthorhombic <br> $a=2.98 \mathrm{~nm}$ <br> $b=10.04 \mathrm{~nm}$ <br> $\gamma=90^{\circ}$ | Orthorhombic <br> $a=2.78 \mathrm{~nm}$ <br> $b=7.85 \mathrm{~nm}$ <br> $\gamma=90^{\circ}$ |
| 3.67 | 1.71 | VS | 06 <br> 15 | 0.15 | 1.674 <br> 1.665 |  | 1.00 |
|  | W | 31 | 0.12 | 0.989 |  |  |  |
| 6.59 | 0.95 | W | 28 | 0.13 | 0.960 |  |  |
| 7.37 | 0.852 | W | 0,12 | 0.13 | 0.837 |  |  |

Table S3: Tentative structure in TATA/TCEH at $20^{\circ} \mathrm{C}$ based on the structure I previously published ${ }^{13}$. $\mathrm{q}_{\text {exp }}, \mathrm{d}_{\text {exp }}, \mathrm{q}_{\text {cal }}, \mathrm{d}_{\text {cal }}$ : experimental and calculated scattering vectors and spacings from peak position; I: intensity of reflection, signal intensity code: $\mathrm{VS}=$ very strong, $\mathrm{S}=$ strong, $\mathrm{W}=$ weak, $h k$ are the Miller indices of the reflections; $a, b, \gamma$, lattice parameters. The lattice parameters of structure I from reference 13 are also given. Basically, only the reflections satisfying $h+k=2 n$ are present.


Figure S2: distance $\mathrm{d}_{\text {calc }}$ calculated with the above unit cell for TATA/TCE $\left(a=2.98 \mathrm{~nm}, b=10.04 \mathrm{~nm}, \gamma=90^{\circ}\right)$ versus the experimental values $d_{\text {exp. }}$. Fit performed with a straight line of fixed slope of 1 and of intercept 0 gives a coefficient of determination $\mathrm{R}^{2}=0.9980$. Conversely, a linear fit with a fixed intercept (0) gives a slope of 1.004, and a coefficient of determination $\mathrm{R}^{2}=0.9998$.

Figure S3: Indexation of the $h k$ planes with the reflections corresponding to $h+k=2 n$.

| $\mathrm{q}_{\exp }\left(\mathrm{nm}^{-1}\right)$ | $\mathrm{d}_{\exp }(\mathrm{nm})$ | $\mathrm{I}(\mathrm{q})$ | $h k$ | $\mathrm{d}_{\text {cal }}(\mathrm{nm})$ from lattice <br> parameters of Structure $\mathrm{I}^{13}$ | Lattice parameters of <br> structure $\mathrm{I}^{13}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 2.449 | 2.56 | VS | 11 | 2.67 | Orthorhombic <br> $a=2.78 \mathrm{~nm}$ <br> $b=7.85 \mathrm{~nm}$ <br> $\gamma=90^{\circ}$ |
| 3.25 | 1.933 | S | 04 | 1.96 |  <br> 4.79 |

Table S4: Diffraction peaks from PVC20/TATA/TCE at $\mathrm{T}=50^{\circ} \mathrm{C}$. Positions of peaks $\mathrm{q}_{\mathrm{exp}}$, and the corresponding distance $\mathrm{d}_{\text {exp }}, \mathrm{I}(\mathrm{q})$ : intensity of reflection, signal intensity code: VS = very strong, $\mathrm{S}=$ strong, $\mathrm{M}=$ middle, the corresponding Miller indices, and $\mathrm{d}_{\text {cal }}$ calculated with the lattice parameter of structure $I^{13}$. Note that the 13 reflection is absent possibly due to a distortion of the unit cell.

