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Hierarchy of Asymmetry at Work: Chain-Dependent Helix-to-Helix Interactions in Supramolecular Polymers

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Abstract: A detailed investigation of the hierarchy of asymmetry operating in the self-assembly of achiral (1) and chiral ((*S*)-2 and (*R*)-3) 1,3,5-triphenylbenzenetricarboxamides (TPBAs) is reported. The aggregation of these TPBAs is conditioned by the point chirality at the peripheral side chains for (*S*)-2 and (*R*)-3. An efficient helix-to-helix interaction that goes further in the organization of fibrillar bundles has been experimentally detected and theoretically supported only for the achiral TPBA 1. The effective interdigitation of the achiral aliphatic side chains produces a social self-sorting to form preferentially heterochiral macromolecular aggregates.

The structure and function of most biopolymers stem from the interaction of their constitutive units at different levels of hierarchy. Initially, the covalent bonding of the building blocks produces a first level of organized backbones. These secondary, chiral structures further interact to yield tertiary and quaternary assemblies. To emulate the construction of such complex structures, supramolecular polymers are being elegantly exploited.^[1,2] A number of helical supramolecular polymers in which the self-assembling units are endowed with stereogenic centers at peripheral side chains have been reported.^[3,4] More scarce are the examples in which different elements of asymmetry (stereogenic centers and/or axial chirality) compete to dictate the helicity of the polymer.^[5] In all them, axial chirality prevails with no influence of the point chirality.^[6,7] At the same time, and despite the examples describing the generation of superhelical fibers from supramolecular polymers,^[8] no clear rules are yet established to go further into the level of hierarchy of the different elements of asymmetry to build up helical supramolecular polymers.

Herein, we report on the self-assembling features of a series of 1,3,5-triphenylbenzenetricarboxamides (TPBAs) endowed with achiral (1) or chiral (*(S)-2* and *(R)-3*) paraffinic side chains (Figure 1a). At the molecular level, the restricted rotation of the benzamide units would afford a propeller-like configuration and, consequently, the generation of the *M* and *P* atropisomers (Figure 1b).^[9] Experimental and theoretical evidences demonstrate that the cooperative supramolecular polymerization

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of 1-3 produces helical columnar stacks in which the molecular atropisomerism is cancelled (Figure 1c). In this first level of hierarchy, the handedness of the helical supramolecular structures is biased by the peripheral stereogenic centers. Importantly, the achiral or chiral nature of the peripheral side chains of 1-3 plays a crucial role in the consecution of a superior level of hierarchical organization. Columnar stacks of TPBA 1 experience an efficient interdigitation through the achiral side chains forming bundles of fibers (Figure 1d). These bundles generate a spontaneous anisotropy spectroscopically visualized by circular (CD) and linear dichroism (LD). In contrast, the branched nature of chiral (S)-2 and (R)-3 impedes the interdigitation and the tertiary level is not achieved. The results presented highlight the hierarchy of different structural elements (point chirality and branched nature of the peripheral side chains) to bias the handedness of the supramolecular helical arrangements, which further determine a tertiary organization level through helix-to-helix interdigitation.



Figure 1. a) Chemical structure of TPBAs **1**, **(S)-2** and **(R)-3**. b) Minimumenergy structure calculated for the two possible atropisomers of TPBA. c) Lefthanded helical columnar arrangement of a decamer of the TPBA model system. d) Illustration of a heterochiral bundle of two helices of **1** formed by the interdigitation of the achiral side chains.

The preparation of TPBAs **1–3** requires a simple multistep protocol, in which a Suzuki cross-coupling between the corresponding 4-(alkylcarbamoyl)phenyl boronic acid and 1,3,5-tribromobenzene is the key step (Scheme S1). All the newly reported compounds were fully characterized by NMR and FTIR

spectroscopy as well as by high-resolution mass spectrometry (see the Supporting Information).

To derive the thermodynamic parameters associated to the supramolecular polymerization of **1**–**3**, variable-temperature UV-Vis (VT-UV-Vis) experiments were performed. A 10 μ M solution of **1** in a mixture of methylcyclohexane/1,2-dichloroethane (MCH/DCE) 95/5 at 20 °C shows a broad absorption centered at 270 nm. This band increases in intensity and slightly shifts bathochromically (272 nm) upon heating the solution to 80°C (Figure S1). The V-shaped cooling curve (Figure S2a), that could be indicative of a hierarchical supramolecular polymerization recently described for referable systems,^[10,11] cannot be fitted neither to a cooperative nor to an isodesmic model.^[2,12] Only by decreasing the concentration to a very low value (5 μ M) it is possible to achieve a non-sigmoidal curve characteristic of a cooperative supramolecular polymerization (Figure S2b).

Similarly to related tricarboxamides, [4d,4e,13,14] the selfassembly of 1 proceeds through the formation of a triple array of hydrogen bonds between the amide groups together with the π stacking of the aromatic as confirmed from concentrationdependent ¹H NMR and FTIR experiments. The former show that the aromatic protons shield and the amide protons shift downfield as concentration increases (Figure S3). In the latter, the N-H and Amide I (C=O) stretching bands as well as the Amide II (C-N) bending band recorded at 3287, 1623, and 1532 cm⁻¹, respectively, indicate the formation of a three-fold intermolecular hydrogen-bonding array (Figure S4).[4d,4e,13,14] Density functional theory (DFT) calculations at the B3LYP-D3/6-31G** level for a TPBA model, in which the long alkyl chains are replaced by methyl groups to reduce the computational cost the Supporting Information), corroborate (see this supramolecular organization. The TPBA molecules form a helical columnar stack in which the monomeric units are one on top of each other rotated by 31° (Figure 1c and S5). To maximize the H-bonding interactions, the amide groups are twisted 36° giving rise to N-H···O=C distances of 2.198 Å, the adjacent molecules in the stack being separated by 3.190 Å. This arrangement favours the planarization of the triphenylbenzene moiety (dihedral angles < 15°).

Theoretical calculations substantiate and give further insight into the cooperative supramolecular polymerization mechanism of **1**. The calculated interaction energy per monomer unit $(E_{int,n})$ in a columnar stack of the TPBA model system corroborates the cooperative character of the self-assembly of 1. Plotting $E_{int,n}$ values against the number of monomeric units results in a hyperbolic curve in which the $E_{int,n}$ grows rapidly until reaching the asymptotic limit (-211 kJ/mol) at around n = 10 units (Figure S6a). The asymptotic behaviour of $E_{int,n}$ is diagnostic of an initial nucleation process, in which the stability of the aggregate rapidly increases with n, followed by an elongation process, in which the incorporation of new monomeric units has no additional effect.^[4c,15] The cooperative self-assembly of 1 is also supported by the increase of the dipole moment per monomer unit (DM_n) calculated for (TPBA)_n aggregates (Figure S6b). The exponential growth of DM_n along the stacking direction implies the enhancement of the polarization of the H-bonding network during the nucleation.[16]

VT-UV-Vis experiments performed with (S)-2 and (R)-3 using the same experimental conditions (MCH/DCE, 95/5) allows deriving all the thermodynamic parameters associated to the supramolecular polymerization of these two chiral TPBAs. Plotting the variation of the molar fraction of aggregates, α_{aggr} , against temperature results in non-sigmoidal curves, diagnostic of a cooperative mechanism (Figure S7). A complete set of thermodynamic parameters can be derived by fitting these curves to the equilibrium (EQ) model (Table S1).^[12] All the thermodynamic parameters are very similar to those reported previously for referable tricarboxamides showing a high degree of cooperativity ($\sigma \sim 10^{-6}$).^[14]



Figure 2. Theoretical simulation of the CD spectra calculated for the *P* and *M* monomers (a) and the left- and right-handed dimers (b) of model TPBA; c) Experimental CD spectra of (S)-2 and (R)-3 (MCH/DCE, 95/5, 10 μM, 298 K).

To disentangle the chiroptical features of the supramolecular assemblies formed by the reported TPBAs, a computational study was performed under the DFT approach (see the Supporting Information). The isolated monomer of model TPBA displays a minimum-energy C_3 geometry in which the

benzamide units are rotated 37° clockwise to yield a propellerlike geometry (Figure 1b and S5a). The rotation in a counterclockwise manner (-37°) results in an isoenergetic mirror-image analogue. The theoretical CD spectra calculated for these two atropisomers show a complex bisignate pattern

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with positive and negative peaks at 304, 275, 249, 207 and 193 nm (Figure 2a). However, the CD spectra computed for *M*- and *P*-type dimers of model TPBA are simpler with bisignate signals peaking at 309 and 268 nm and a zero-crossing point at 290 nm (Figure 2b). These bisignate CD bands originate from high-energy electronic excitations involving the aromatic TPBA core (Figure S8), and their sign is dictated by the handedness of the dimer.

The experimental CD spectra of (S)-2 and (R)-3 show a clear bisignate Cotton effect with maxima at 281 and 258 nm and a zero-crossing point at 270 nm (Figure 2c and S9a). By comparison with the simulated CD spectra of the dimeric species, the self-assembly of (S)-2 and (R)-3 can be unequivocally assigned to right- and left-handed helical structures, respectively, in good agreement with previous results for related tricarboxamides.^[4c,4d,13] Note that the dichroic pattern of (S)-2 and (R)-3 is much simpler than that predicted for the TPBA monomer (Figure 2a) due to the planarization experienced by the benzenes around the central ring upon selfassembly (Figure 1c and S5). This planarization cancels the molecular atropisomerism switching the hierarchy of asymmetry. In this case, and unlike previous examples in which atropisomerism prevails over point chirality,[5-7] the chiral information embedded in the stereogenic centers of the side chains biases the handedness of the helical stacks in our TPBAs.

The thermodynamic characterization of the supramolecular polymerization of TPBAs **1–3** was undertaken by performing experiments of amplification of chirality.^[3] Sergeants-and-soldiers experiments were first carried out by adding increasing amounts of chiral **(S)-2** into achiral **1** keeping constant the total

concentration (c_7). Surprisingly, the addition of the sergeant (S)-2 results in dichroism spectra of different shape and intensity for the different mixtures (Figure S10). These findings could be indicative of a strong trend of 1 to form fibrillar structures that bundle into thick filaments with a concomitant macroscopic alignment of such filaments.^[17] To document this macroscopic alignment and the subsequent anisotropy generated in the cuvette, the CD spectra of 1 was registered in MCH/DCE 95/5 at c_T = 10 µM. The CD spectrum, that resembles to that obtained for (R)-3, slightly increases upon rotary stirring (Figure 3a). In addition, heating this solution at 80 °C followed by a rapid cooling on an ice bath results in a mirror-like CD spectrum of higher intensity (Figure S11). This inversion of the helicity could be indicative of a pathway complexity in the self-assembly of the sample.^[18] However, this is not the case because the CD spectrum is strongly contaminated by a LD response that decreases upon rotary stirring (Figure 3a, inset). This unexpected dichroic behaviour of 1 is comparable to that observed previously for some other achiral self-assembling units and is attributed to the strong trend to form fibillar structures and also to the chiral alignment of the fibers in solution as a consequence of convective flows in the measuring cuvette.^[17,19] Interestingly, this is not the case of chiral (S)-2 and (R)-3 that do not present any LD contamination of the CD spectra (Figure S9b). The fibrillar nature of the aggregates formed from 1 was visualized by atomic force microscopy (AFM) on mica as surface. The AFM images show a dense network of thick filaments (tens of nanometers) forming rope-like structures constituted by the aggregation of thinner fibrils (Figure 3b and S12).



Figure 3. a) CD spectra of TBPA 1 (10 μ M; MCH/DCE, 95/5, 20 °C). The inset shows the corresponding LD spectra; b) Phase AFM image of the fibrillar structures of 1 onto mica (*z* scale = 65 nm); c) Changes in CD intensity as a function of e.e. upon adding (*S*)-2 to a solution of (*R*)-3 (MCH, 293 K, c = 25 μ M); e.e. = 1 and e.e. = -1 correspond to pure (*S*)-2 and (*R*)-3, respectively. The inset shows the changes in the corresponding CD spectra.

Majority rules experiments, performed by adding dissimilar amounts of the (*S*)-2 and (*R*)-3 enantiomers keeping c_{T} constant, were carried out to complete the thermodynamic characterization of the supramolecular polymerization of (*S*)-2 and (*R*)-3. The non-linear variation of the dichroic response was fitted to the two-components EQ model to extract the mismatch enthalpy (ΔH_{mm}).^[12] This energetic term, calculated to be -1.00 kJ/mol (Table S1), indicates the penalization undergone by the system upon incorporating a monomer into an aggregate of its unpreferred helicity. The ΔH_{mm} value is smaller to that derived for related C_3 -symmetric tricarboxamides,^[12.13] and gives rise to an efficient amplification of chirality: with only 22% of enantiomeric excess (e.e.), the chirality of the mixture is the same as that observed for pristine (S)-2 or (R)-3.

Finally, we attempted to rationalize the helix-to-helix interactions present in the fibrillar bundles observed

experimentally for 1 by using theoretical simulations. The geometry of TPBAs 1 and (S)-2 was obtained from DFT calculations (Figure S13). From these monomeric units, helical icosamers were constructed and optimized at the molecular mechanics level for both 1 and (S)-2 (Figure S14). The rotation angle (ca. 30°) between adjacent monomers results in a supramolecular cavity suitable to induce efficient van der Waals interactions between the aliphatic side chains of vicinal aggregates. Particularly interesting is the case of 1 in which two different helix-to-helix interactions can be postulated considering that this achiral monomeric unit yields a racemic mixture of both right- and left-handed helical structures. The first of these two possibilities implies a self-recognition or narcissistic self-sorting phenomenon in which the two enantiomeric structures interact with those of the same species to form homochiral superstructures (Figure 4a). The second possibility implies a self-discrimination or social self-sorting in which P- and M-type helices interact to form a heterochiral aggregate (Figure 4b).^[20] For chiral (S)-2, the transference of the point chirality embedded in the side chains provokes the formation of P-type helices, and only a narcissistic self-sorting is possible through homochiral helix-to-helix interactions (Figure 4c).



Figure 4. Top and side views of density maps of homochiral (a) and heterochiral (b) helix-to-helix interactions in 1 and homochiral helix-to-helix interaction in (S)-2 (c). The distance between the two column centers is indicated in the top view.

The unbranched achiral side chains in 1 allow for an efficient between homochiral columns interdigitation with an intercolumnar distance of 28.3 Å (Figure 4a and S15) and an intercolumnar interaction energy (E_{int,col}) of -316 kJ/mol. Importantly, the intercolumnar interaction is maximized when two columns of 1 with different handedness interdigitate (Figure 4b and S16), leading to a column-to-column distance of only 25.4 Å and an E_{int,col} of -482 kJ/mol. In contrast, the branched nature of the peripheral aliphatic chains in chiral (S)-2 impedes an adequate interdigitation between the two columns (Figure 4c, S17 and S18), and a large intercolumnar distance of 32.4 Å with a small E_{int.col} of -98 kJ/mol is predicted for the homochiral superstructure. The helix-to-helix stabilization in the macromolecular dimers originates from weak van der Waals contacts, and a pleasant correlation between the intercolumnar contact area (ICA) and the $E_{int,col}$ values is obtained (Table S2 and Figure S19). The complementary supramolecular pockets calculated for the social self-sorting of 1 result in efficient helix-to-helix interactions that justify the macroscopic alignment of supramolecular columns in fibers. This is not the case of chiral **(S)-2** in which the helix-to-helix interaction is much weaker.

To summarize, we report on the self-assembling features of new series of C_3 -symmetric TPBAs 1–3. A detailed а experimental and theoretical study of the hierarchy of asymmetry elements operating in the formation of right- or lefthanded supramolecular polymers is provided. The restricted rotation of the lateral benzamide units yields a mixture of P- and M-type atropisomers in the molecularly dissolved state. The supramolecular polymerization of these units by H-bonding and π-stacking interactions cancels this atropisomerism, and the next level of hierarchy is biased by the point chirality of the peripheral side chains. An efficient helix-to-helix contact is for the achiral TPBA 1 to go further in the macromolecular organization of tertiary superstructures. Theoretical calculations demonstrate that the efficient interdigitation of the achiral aliphatic chains affords a social self-sorting effect to form preferentially heterochiral bundles. The results presented herein contribute to shed light on the rules governing the transformation of secondary into tertiary supra- and macromolecular structures and take a step forward in understanding the hierarchy of the elements of asymmetry to bias the handedness of the resulting helical supramolecular polymer.

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COMMUNICATION

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