Chiral Cyclobutane β-Amino Acid-Based Amphiphiles: Influence of cis/trans Stereochemistry on Condensed Phase and Monolayer Structure

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New diastereomeric non-ionic amphiphiles, cis- and trans-1, based on a cyclobutane beta-amino ester moiety have been investigated to gain insight in the influence exerted by cis/trans stereochemistry and stereochemical constraints on the physicochemical behavior, molecular organization, and morphology of their Langmuir monolayers and dry solid states. All these features are relevant to the rational design of functional materials. Trans-1 showed a higher thermal stability than cis-1. For the latter, a higher fluidity of its monolayers was observed when compared with the films formed by trans-1 whose BAM images revealed the formation of condensed phase domains with a dendritic shape, which are chiral and all of them feature the same chiral sign. Although the formation of LC phase domains was not observed by BAM for cis-1, compact dendritic crystals floating on a fluid subphase were observed beyond the collapse, which are attributable to multilayered 3D structures. These differences can be explained by the formation of hydrogen-bonds between the amide groups of consecutive molecules allowing the formation of extended chains for trans-1 giving ordered arrangements. However, for cis-1, this alignment coexists with another one that allows the simultaneous formation of two hydrogen bonds between the amide and the ester groups of adjacent molecules. In addition, the propensity to form intramolecular hydrogen-bonds must be considered to justify the formation of different patterns of hydrogen-bonding and, consequently, the formation of less ordered phases. Those characteristics are congruent also with the results obtained from SAXS-WAXS experiments which suggest a more bent configuration for cis-1 than for trans-1.

Acknowledgment: We thank Jaume Caelles, in the SAXS-WAXS service at IQAC, for X-Ray measurements; and Dr. Fabrizio Marinelli for the optimization of the dimeric structures in Figure 7. Financial support from MINECO (grants CTQ2013-41514-P, and CTQ2013-43754-P) is gratefully acknowledged. Authors also thank the support from Generalitat de Catalunya (2014SGR358 and 2014SGR836).