

^2H and ^{13}C NMR-Based Enantiodetection Using Polyacetylene versus Polypeptide Aligning Media: Versatile and Complementary Tools for Chemists



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Invited for this month's cover are the collaborating groups of Dr. Philippe Lesot (DR CNRS) at Université Paris-Sud/Université Paris-Saclay, France, and Professor Michael Reggelin at TU Darmstadt, Germany. The cover shows the proton-decoupled natural abundance deuterium (NAD- $\{^1\text{H}\}$) Q-resolved Fz 2D-NMR spectrum of (\pm)-3-methylhexane measured in the anisotropic lyotropic chiral liquid-crystalline phase formed by a concentrated solution of a helically chiral polyarylacetylene in chloroform solvent. Seventeen out of the twenty possible deuterium quadrupolar doublets are observed, demonstrating the enormous enantiodifferentiating capability of the system, even for an unfunctionalized chiral alkane. Read the full text of the article at 10.1002/cplu.201800493.

What prompted you to investigate this problem?

Dr. Lesot (DR CNRS) from the Paris-Sud/Paris-Saclay University (FR) and Prof. Reggelin from Darmstadt University (DE) are interested in the global understanding of the mechanisms/phenomena of NMR-spectroscopic enantiodifferentiation being operative in chiral lyotropic liquid-crystalline (LLC) phases made of glutamate-derived polypeptide (PBLG) and/or valine-derived polyacetylene (PLA) helically chiral polymers. One important challenge of this work was to establish the analytical potential of deuterium residual quadrupolar couplings (^2H -RQCs) (on deuterated analytes and at natural abundance level (NAD NMR)) for enantiodiscrimination applications that, so far, have never been measured and exploited in the polyacetylene-based oriented systems.

What is the most significant result of this study?

The first experimental results using NAD 2D-NMR spectroscopy in PLA, previously widely used in PBLG mesophases, appear very promising because they demonstrate remarkable analytical potential for spectroscopic enantiodiscrimination purposes, including the difficult case of an unfunctionalized chiral alkane for which the conventional, isotropic NMR approaches give generally poor results or fail (see the cover picture). Through our new findings appealing prospects are now open.

How did the different team members contribute?

Lesot's group performed the anisotropic NMR spectroscopy and the synthesis of numerous deuterated analytes investigated, whereas Reggelin's group prepared the polyacetylene-based liquid crystals (D and L configuration) using a new optimized synthetic strategy.

What do you consider exciting developments in the field?

To reach the final goal, namely the determination of absolute configuration of chiral molecules by NMR, it is necessary to develop new enantiodiscriminating chiral anisotropic media and to understand how they differentiate enantiomers. Moreover, the combination of different polymer structures as described in this article should offer new appealing opportunities for the application of these chiral media in anisotropic NMR.

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