**NMR RELAXATION IN DENDRIMERS**

Denis A. Markelov1, Maxim Dolgushev2 , Erkki Lahderanta3

1St. Petersburg State University

2Institute of Physics, University of Freiburg

3Laboratory of Physics, Lappeenranta University of Technology

markeloved@gmail.com

This report focuses on recent advances in the theory of local orientational mobility in dendrimers that reveals in the NMR relaxation [1]. In particular, we summarize recent results of analytic theory [2-3], computer simulations [4-6], and NMR relaxation experiments [7]. The analytic theory provides basic means for the analysis of the simulations and experiments by predicting the existence of two dominating processes: overall branch relaxation and local vibrations. On the other hand, the results of simulations and experiments complete the picture by a third process of rotation of the dendrimer as a whole.

The NMR relaxation reveals a fundamental importance of the local constraints on segments’ orientations. Remarkably, the model, in which such constraints are absent, overestimates local vibrations making the NMR relaxation rate functions for segments that have different topological location in the dendrimer to be practically indistinguishable. Inclusion of the bending rigidity fixes this flaw by endorsing the process of overall branch relaxation. This leads to a correct recognition of the slower mobility of the segments that are located closer to the dendrimer’s core. The crucial role of the local constraints for the NMR relaxation functions is supported by a series of experiments and simulations.

[1] D.A. Markelov, M. Dolgushev, E. Lähderanta, Annu. Rep. NMR Spectrosc. 91 (2017) 1

[2] Y.Y. Gotlib, D.A. Markelov, Polym. Sci. Ser. A. 49 (2007) 1137

[3] D.A. Markelov, M. Dolgushev, Y.Y. Gotlib, A. Blumen J. Chem. Phys. 140 (2014) 244904

[4] D.A. Markelov, Y.Y. Gotlib, A.A. Darinskii, A. V Lyulin, S. V Lyulin, Polym. Sci. Ser. A. 51 (2009) 331–339

[5] D.A. Markelov, S.G. Falkovich, I.M. Neelov, M.Y. Ilyash, V. V. Matveev, E. Lähderanta, P. Ingman, A.A. Darinskii, Phys. Chem. Chem. Phys. 17 (2015) 3214

1 D.A. Markelov, A.N. Shishkin, V.V. Matveev, A.V. Penkova, E.Lähderanta, V.I. Chizhik Macromolecules. 49 (2016) 9247

[7] L.F. Pinto, J. Correa, M. Martin-Pastor, R. Riguera, E. Fernandez-Megia, J. Am. Chem. Soc. 135 (2013) 1972