Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Ortho-para conversion of endohedral water in the fullerene C_{60} at cryogenic temperatures[1] ANNA SHUGAI, U. NAGEL, T. RÕÕM, NICPB, Tallinn, Estonia, S. MAMONE, M. CONCISTRÈ, B. MEIER, A. KRACHMAL-NICOFF, R.J. WHITBY, M.H. LEVITT, Chemistry, Uni. of Southampton, UK, XUEGONG LEI, YONGJUN LI, N.J. TURRO, Dep. of Chemistry, Columbia Uni., New York — Water displays the phenomenon of spin isomerism in which the two proton spins either couple to form a triplet (ortho water, $I = 1$) or a singlet nuclear spin state (para water, $I = 0$). Here we study the interconversion of para and ortho water. The exact mechanism of this process is still not fully understood. In order to minimize interactions between molecules we use a sample where a single H_2O is trapped in the C_{60} molecular cage ($H_2O@C_{60}$) and $H_2O@C_{60}$ is crystallized. $H_2O@C_{60}$ has long-lived ortho state [Beduz et al., PNAS **109**, 12894 (2012)] and ortho-para conversion kinetics is non-exponential at LHeT [Mamone et al, J.Chem.Phys. **140**, 194306, (2014)]. We studied mixtures of $H_2O@C_{60}$, $D_2O@C_{60}$ and C_{60} using IR absorption, NMR and dielectric measurements. We saw the speeding up of the interconversion with the growth of $H_2O@C_{60}$ concentration in C_{60} or when $D_2O@C_{60}$ was added. At some temperatures the kinetics is exponential. Models are discussed in order to explain the T and concentration dependence of ortho-para interconversion kinetics.

[1] This work was supported by institutional research funding IUT23-3 of the Estonian Ministry of Education and Research.

Anna Shugai
National Institute of Chemical Physics and Biophysics

Date submitted: 13 Nov 2014

Electronic form version 1.4