Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

The origin of the extremely different solubilities of polyethers in water AMBUJ TIWARI, MARTIJN TROS, BERND ENSING, Van t Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands, JOHANNES HUNGER, MISCHA BONN, Max Planck Institute for Polymer Research, Department of Molecular spectroscopy, Ackermannweg 10, 55128 Mainz, Germany, GERTIEN SMITS, Swammerdam Institute for Life Sciences, University of Amsterdam, Science Park 904, 1098XH Amsterdam, The Netherlands, DANIEL BONN, Institute of Physics, University of Amsterdam, The Netherlands, SANDER WOUTERSEN, Van t Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands — Abstract: The solubilities of polyethers in water are surprisingly counter-intuitive. The best-known example is the difference between polyethylene glycol ([-CH_2-CH_2-O-]$_n$) which dissolves up to 0.5 kg/l, and polyoxymethylene ([-CH_2-O-]$_n$) which is *completely insoluble* in water, exactly the opposite of what one expects from the ratio of hydrophobic to hydrophilic parts in these molecules. Similar anomalies exist for oligomeric and cyclic polyethers. To solve this apparent mystery, we use femtosecond vibrational and GHz dielectric spectroscopy with complementary *ab initio* calculations and molecular dynamics simulations. We find that the dynamics of water molecules solvating polyethers is fundamentally different depending on their C/O composition. The calculations and simulations show that this because the partial charge on the O atoms depends on the number of C atoms by which they are separated. Our results show that quantum effects can have a major impact on aqueous solubilities.

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Date submitted: 20 Nov 2016 Electronic form version 1.4