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Dynamics of bound water molecules in fullerenol at different hydration levels[1] YILIN WANG, University of Maryland, College Park, STEVEN ROBEY, National Institute of Standards and Technology, JANICE REUTT-ROBEY, University of Maryland, College Park — Fullerenols, polyhydroxylated fullerenes, are of great interest as promising materials in medical application because of their high water solubility and biocompatibility. Fullerenols are highly responsive to their environment, for example, they readily undergo hydration under ambient conditions. Understanding the dynamics of water molecules bound to fullerenols, and the interplay between water molecules and fullerenols is important in realizing biological function. Here, broadband dielectric spectroscopy (BDS), was performed on a fullerenol with 44 hydroxyl groups, C60(OH)44, between 300 K and 340 K. At room temperature and under ambient conditions, C60(OH)44 is hydrated, releasing bound water molecules with increasing temperature, as quantified by thermal gravimetric analysis (TGA) measurements. At room temperature, a dielectric band due to collective bulk-like dynamics of the bound water molecules is observed. The relaxation peak of the water molecules shifts to higher frequency with increasing of temperature, reflecting the dynamics of bound water. Upon loss of water molecules, either thermally induced or vacuum induced, the relaxation peak shifts to lower frequency. The stoichiometric relationship between the dielectric properties of the hydrated fullerenol and the interplay between the bound water molecules and C60(OH)44 will be discussed.

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