Methyl tert-Butyl Ether-Water Interactions. (S02-bailey111918-Poster)

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Abstract:

Methyl tert-butyl ether (MTBE) is a well-known environmental contaminant owing to its high solubility in water. Since the early 1990s, MTBE has been added to gasoline to improve air quality in some metropolitan areas of the United States. Improved air quality was, however, achieved at the expense of MTBE tainted water. MTBE from leaking underground gasoline tanks, urban runoff, boats, etc., has been contaminating surface water and ground water in the very areas MTBE use was supposed to improve air quality. Molecular association between MTBE and water is predominantly via hydrogen bonding with water acting as the hydrogen bond donor and MTBE as the hydrogen bond acceptor. The objective of this study is to estimate the strength of the hydrogen bond between MTBE and water, and to determine the structure of the MTBEwater clusters by means of high-level ab initio quantum mechanical and density functional theory calculations. The geometrical structures, vibrational frequencies, and stabilization energies of the MTBE-water complexes are fully corrected for basis set superposition error (BSSE).

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