

Equilibrium hydrogen and oxygen isotope fractionation between water ice and vapor

XIAOBIN CAO^{1*}, HUIMING BAO¹, YUN LIU², JIANWEI WANG¹, JUSTIN A. HAYLES^{1,3}, YONGBO PENG¹, AND BISWAJIT SANTRA⁴

¹ Department of Geology & Geophysics, Louisiana State University; xcao@lsu.edu

² Institute of Geochemistry, Chinese Academy of Sciences

³ Department of Earth Science, Rice University

⁴ Department of Chemistry, Princeton University

The stable isotope compositions of water molecules (i.e. D/H, ¹⁸O/¹⁶O, ¹⁷O/¹⁶O) are diagnostic tools for studying the current and past hydrologic cycle on Earth and other planetary bodies. The equilibrium isotope fractionation factors between ice and vapor (i.e. ^D α , ¹⁸ α , and ¹⁷ α) are some of the fundamental parameters that govern the observed variations in isotope compositions. However, discrepancies among different experimentally or theoretically determined α s exist and the accompanied, highly informative, equilibrium triple oxygen isotope exponent θ ($\theta \equiv \ln^{17}\alpha/\ln^{18}\alpha$) is rarely available. Furthermore, extrapolating experimental results determined at temperatures from -40°C to 0°C to a temperature as low as -150°C has been necessary for studying hydrologic cycle on other planetary bodies such as Mars. However, the validity of this extrapolation still requires investigation. Here, we calculate water isotope fractionation parameters using density functional theory in which the *Ih* ice is represented by a molecular cluster and the anharmonic correction is applied to the isotope effect calculation.