ARTICLE TYPE

Electronic Supplementary Information

contains supplementary figures



Fig. 1 DFTB harmonic (dashed lines) and 10 K BOMD/DFTB anharmonic (plain lines) vibrational spectra of $(H_2O)_2$



Fig. 2 Unscaled DFT M06-2X/d95v(d,p) harmonic infrared spectra of low-energy isomers of $(C_{24}H_{12})(H_2O)$ and $(C_{24}H_{12})(H_2O)_2$



Fig. 3 DFTB harmonic (dashed lines) and 10 K BOMD/DFTB anharmonic (plain lines) vibrational spectra of $(C_{24}H_{12})(H_2O)$



Fig. 4 DFTB harmonic (dashed lines) and 10 K BOMD/DFTB anharmonic (plain line) vibrational spectra of $(C_{24}H_{12})(H_2O)_2$



Fig. 5 Optimised geometries of $(H_2O)_2$ and $(C_6H_6)(H_2O)$ obtained at the MP2 / Aug-cc-pvtz level of theory