Supplementary information: Observation of metastable structures of the dimer of ethylene glycol-water dimer in helium nanodroplets

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1. Mass Spectrometry

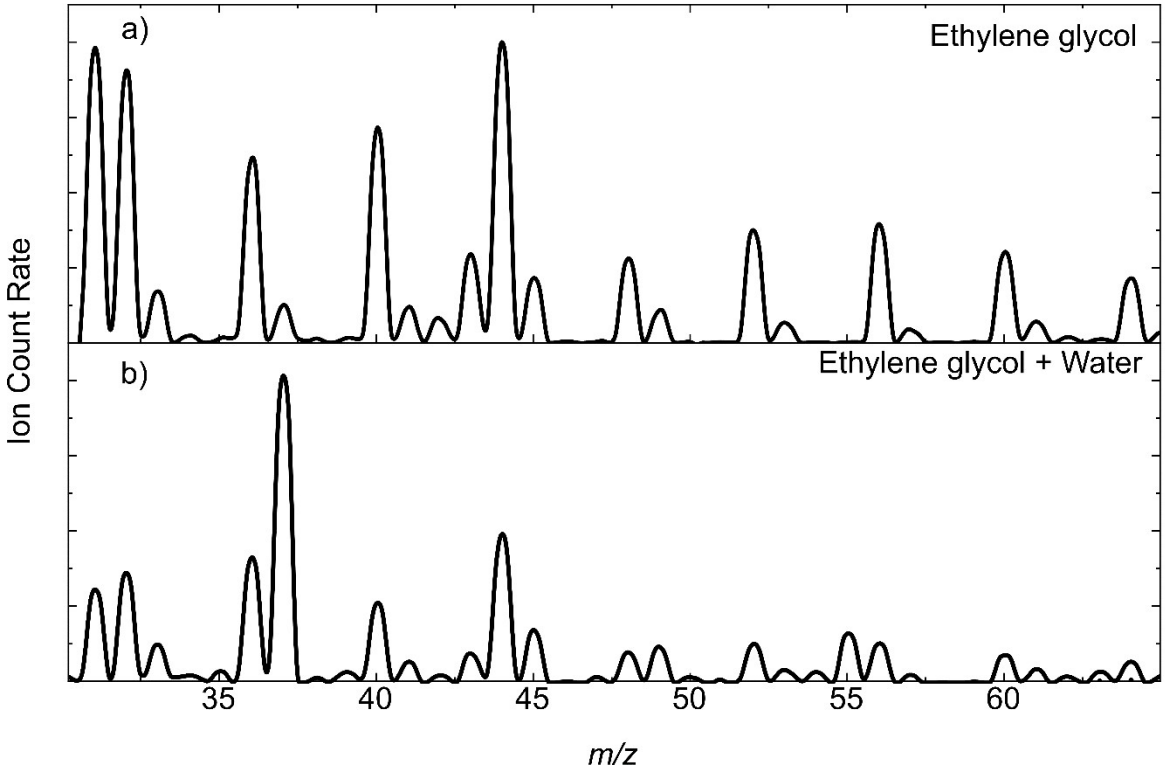

Figure S1. Uncorrected mass spectrum from 30-65 *m/z* for addition of (a) ethylene glycol and (b) ethylene glycol and water to helium nanodroplets.

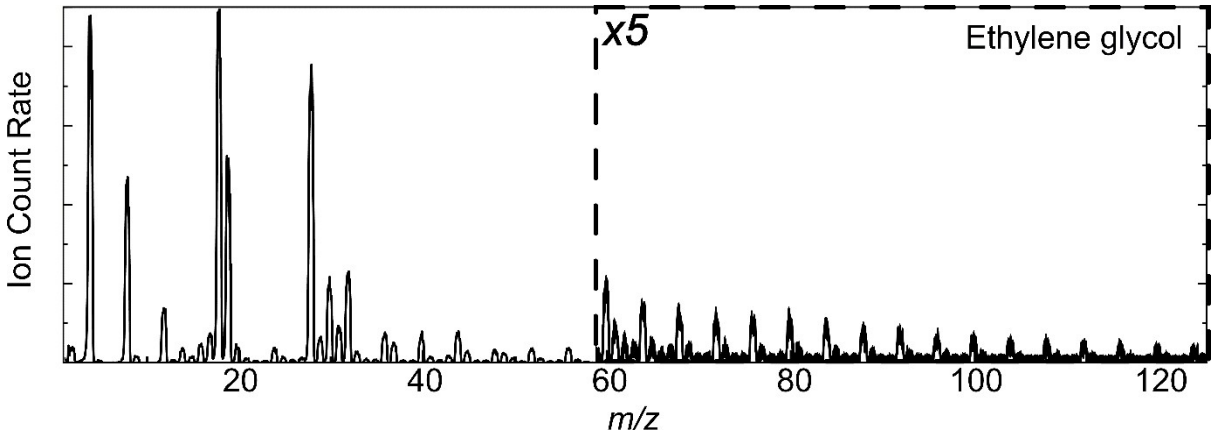

Figure S2. Uncorrected mass spectrum from 1-125 *m/z* for addition of ethylene glycol to helium nanodroplets.

2. Supplementary Spectroscopy

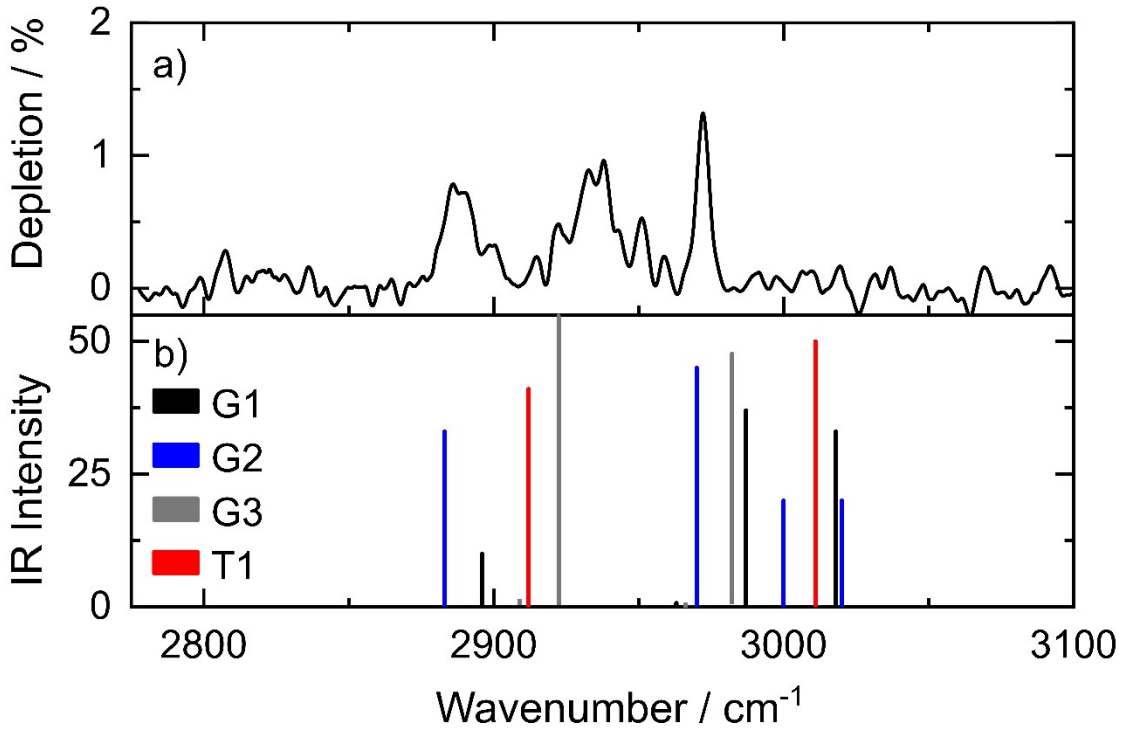

Figure S3. (a) The IR depletion spectrum in the CH stretching region obtained from ethylene glycol in helium nanodroplets. (b) The calculated anharmonic vibrational spectrum for the four lowest energy conformers. Structures of the four conformers are shown in Figure 2c-f of the main text.

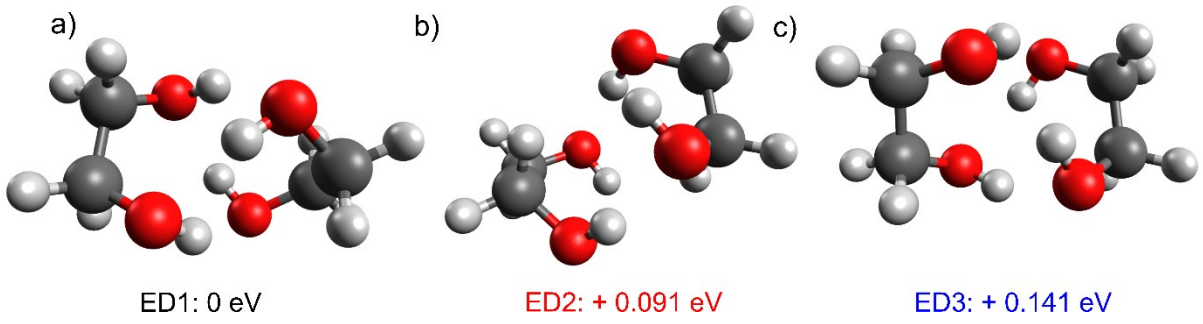

Figure S4. Optimized geometries for ethylene glycol dimers, $(EG)_2$. Energies are shown relative to the minimum energy structure.

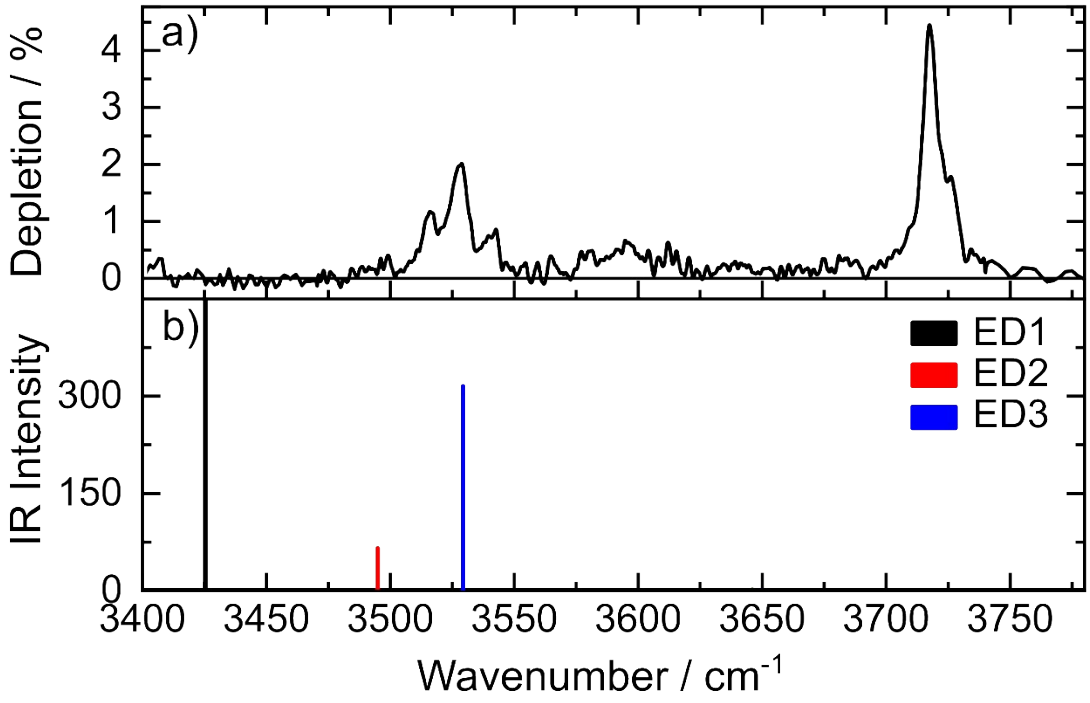

Figure S5. Panel a) is reproduced from Figure 3 of the main text and shows the IR spectrum obtained from helium droplets containing ethylene glycol and water. In panel b) are calculated anharmonic IR spectra for the three conformers found in calculations on ethylene glycol dimer shown in Figure S3. With the exception of ED3, the agreement between theory and experiment is poor. Although there is a peak in the calculated spectrum of ED3 that matches one seen in the experimental spectrum, the absence of these peaks when no water is added confirms that ethylene dimer does not contribute in the experiments.

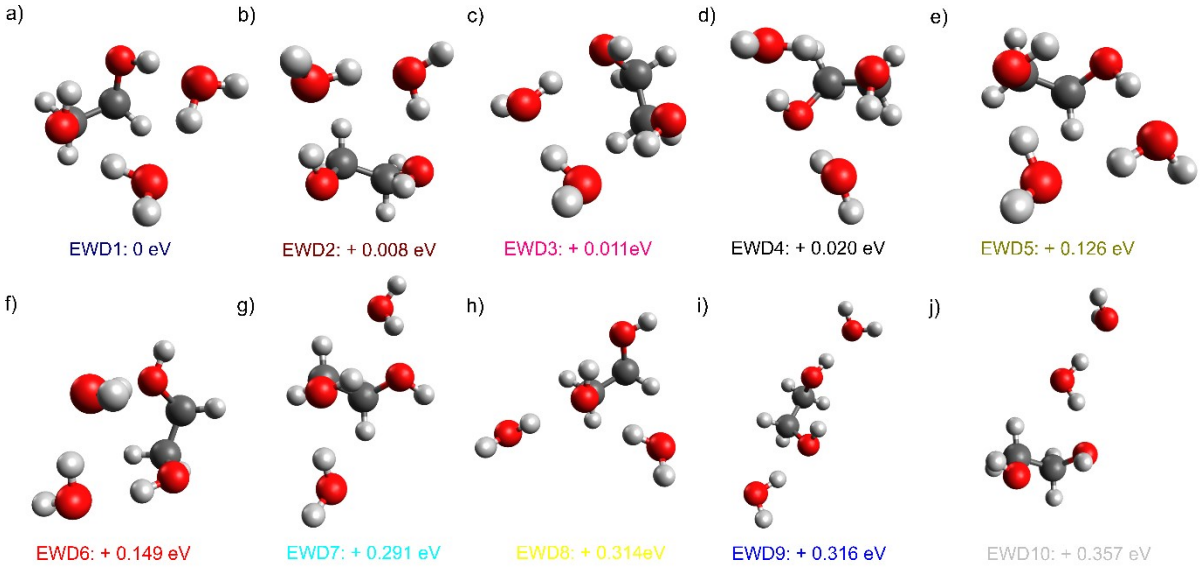

Figure S6. Optimized geometries for an ethylene glycol molecule in the G1 conformer clustered with two water molecules. Energies are shown relative to the minimum energy structure.

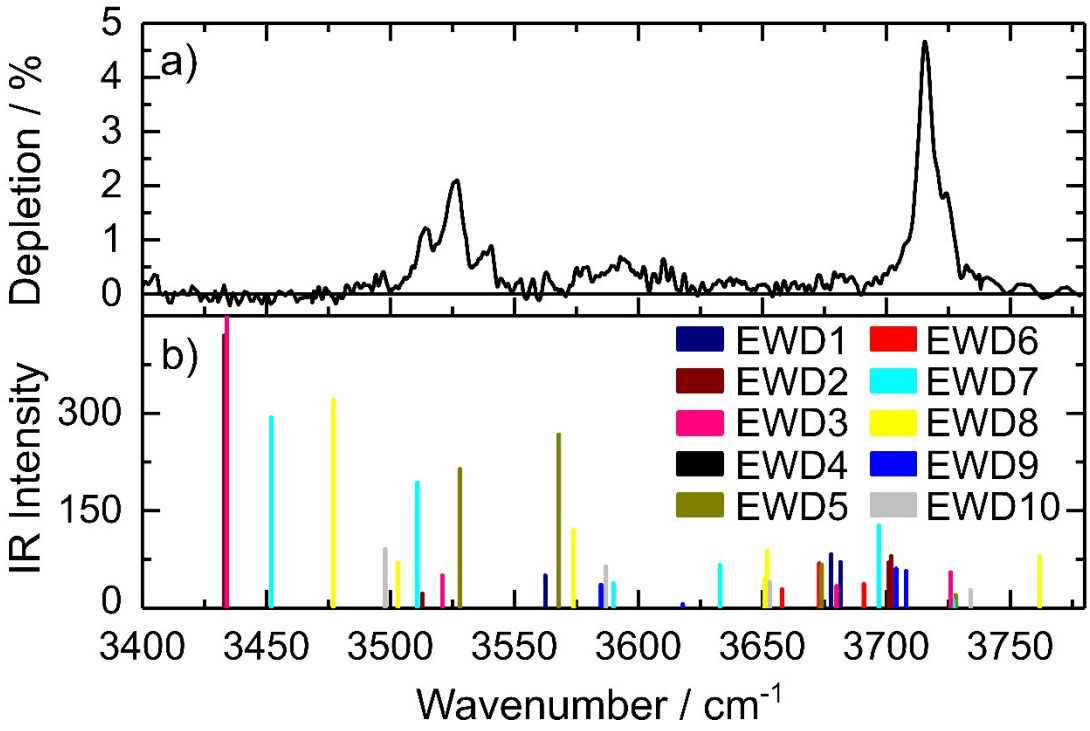

Figure S7. Panel a) is reproduced from Figure 3 of the main text. In panel b) we show the predicted anharmonic vibrational spectra for the ten EG$(H_2O)_2$ conformers shown in Figure S5.

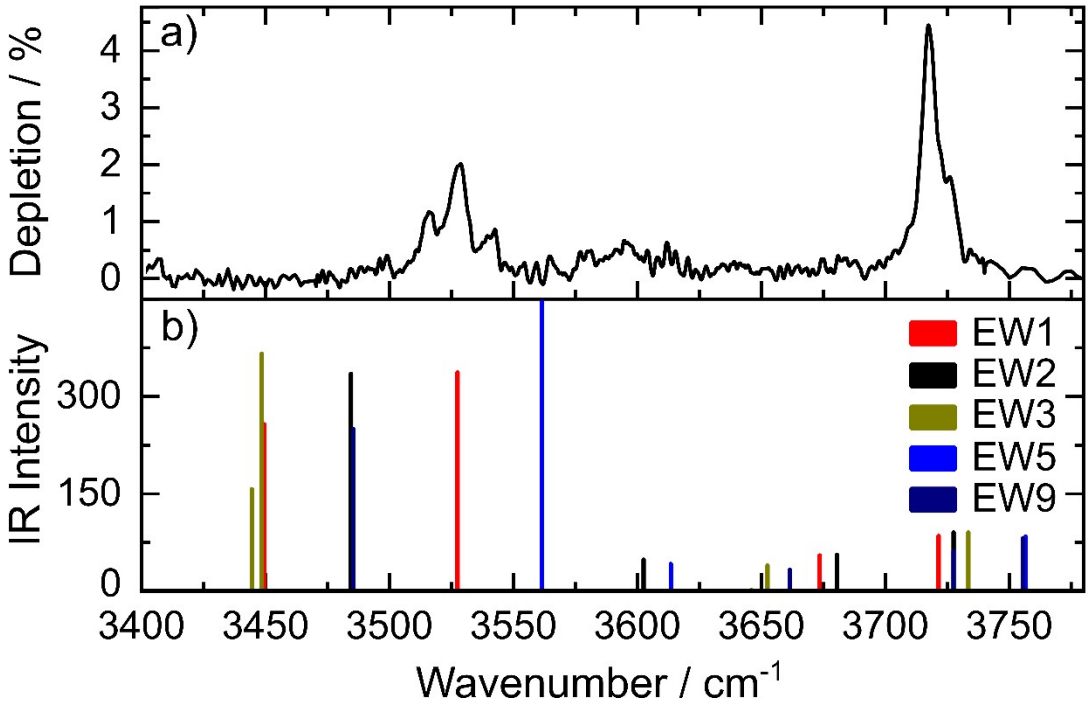

Figure S8. Panel a) is reproduced from Figure 3 of the main text. In panel b) we show the predicted anharmonic IR spectra for the five conformers of EG-H_2O eliminated from the spectral assignment in the main text. Although the global energy minimum, EW1, shows peaks close to those seen in the experimental spectrum, it is also predicted to show an additional and strong peak close to 3450 cm^{-1}. The absence of this peak in the experimental spectrum eliminates this isomer as a possible contributor.