Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular gels in the gas phase? Gelator-gelator and gelator-solvent interactions probed by vibrational spectroscopy.

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Supplementary information.

Figure S1-a. Calculated spectra and structure of the most stable conformers of BzGlc compared to the IRID spectrum. For each conformer, the relative potential energy is given first and the relative 300 K free energy is given below, in KJ/mol.

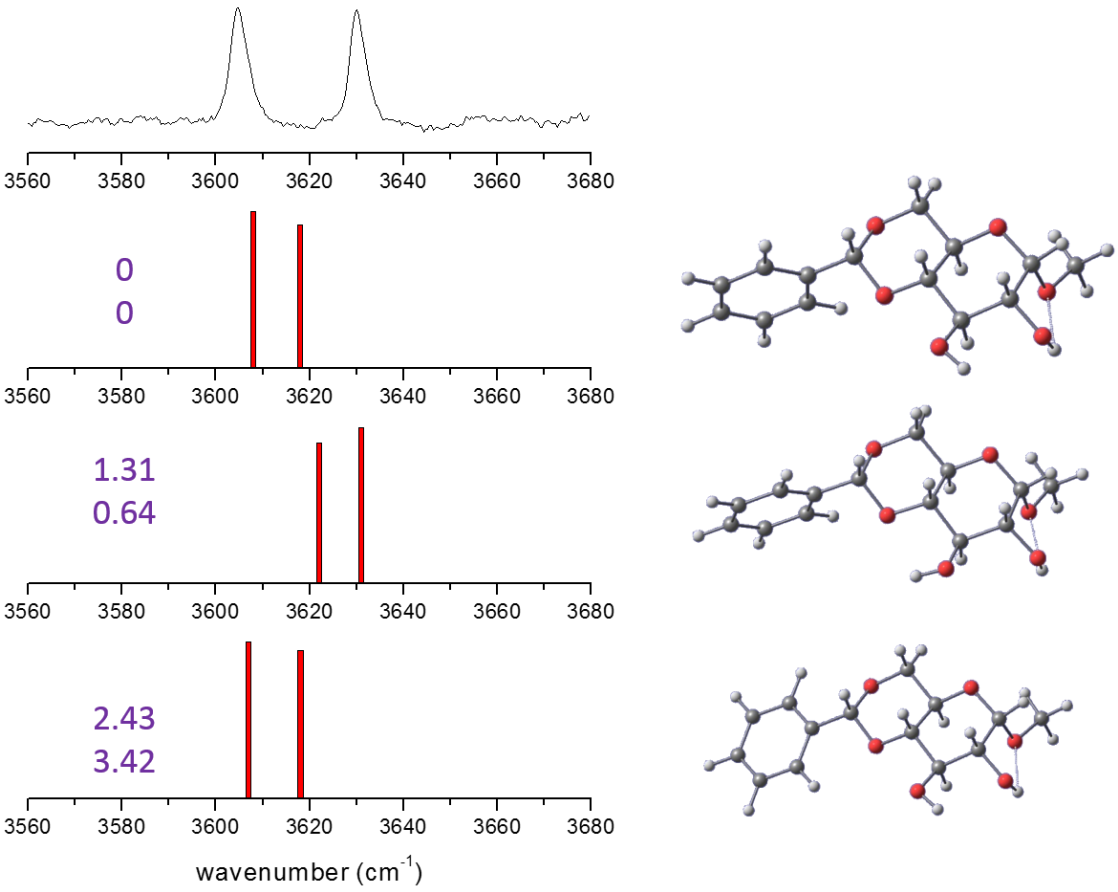

Figure S1-b. Calculated spectra and structure of the most stable conformers of BzGlc compared to the IRID spectrum, continued. For each conformer, the relative potential energy is given first and the relative 300 K free energy is given below, in KJ/mol.

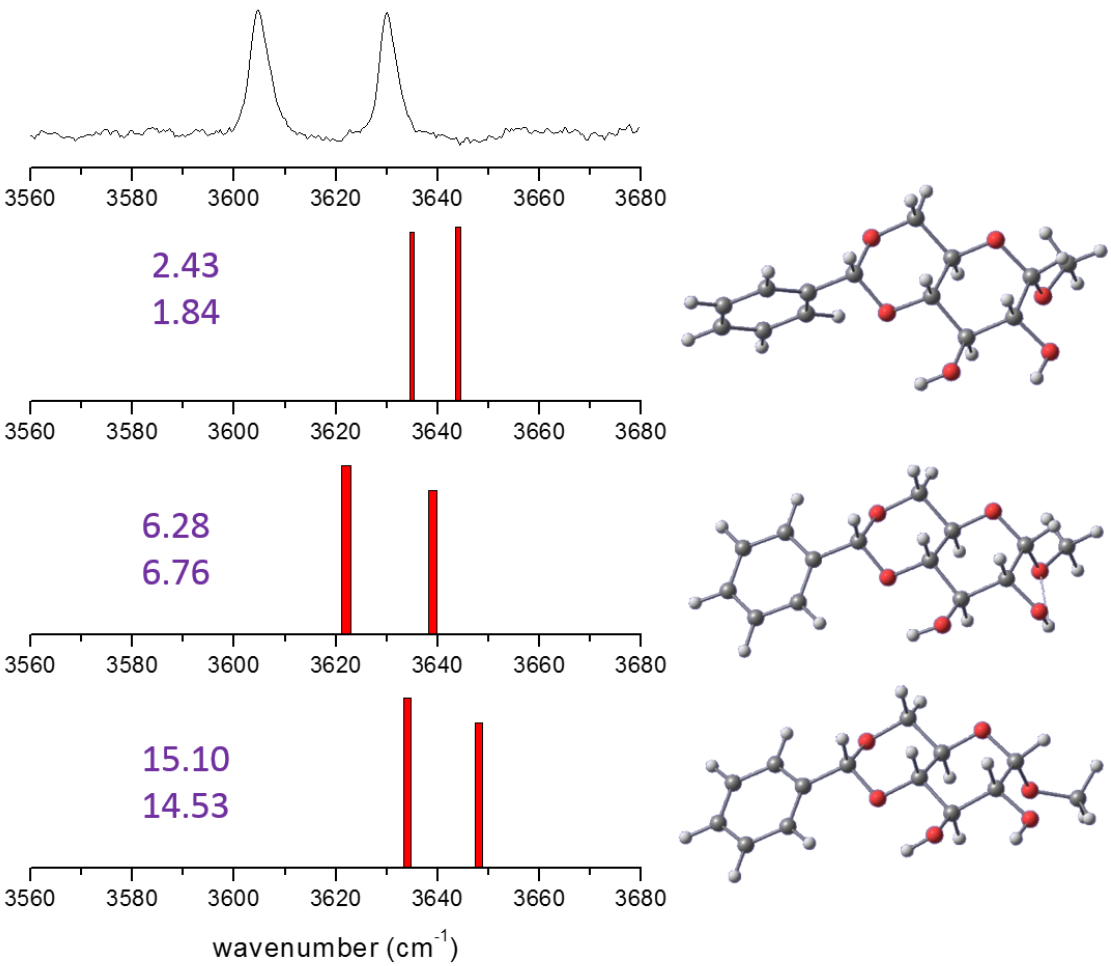

Figure S2-a. Calculated spectra and structure of the most stable conformers of BzGlc-W compared to the IRID spectrum. For each conformer, the relative potential energy is given first and the relative 300 K free energy is given below, in KJ/mol.

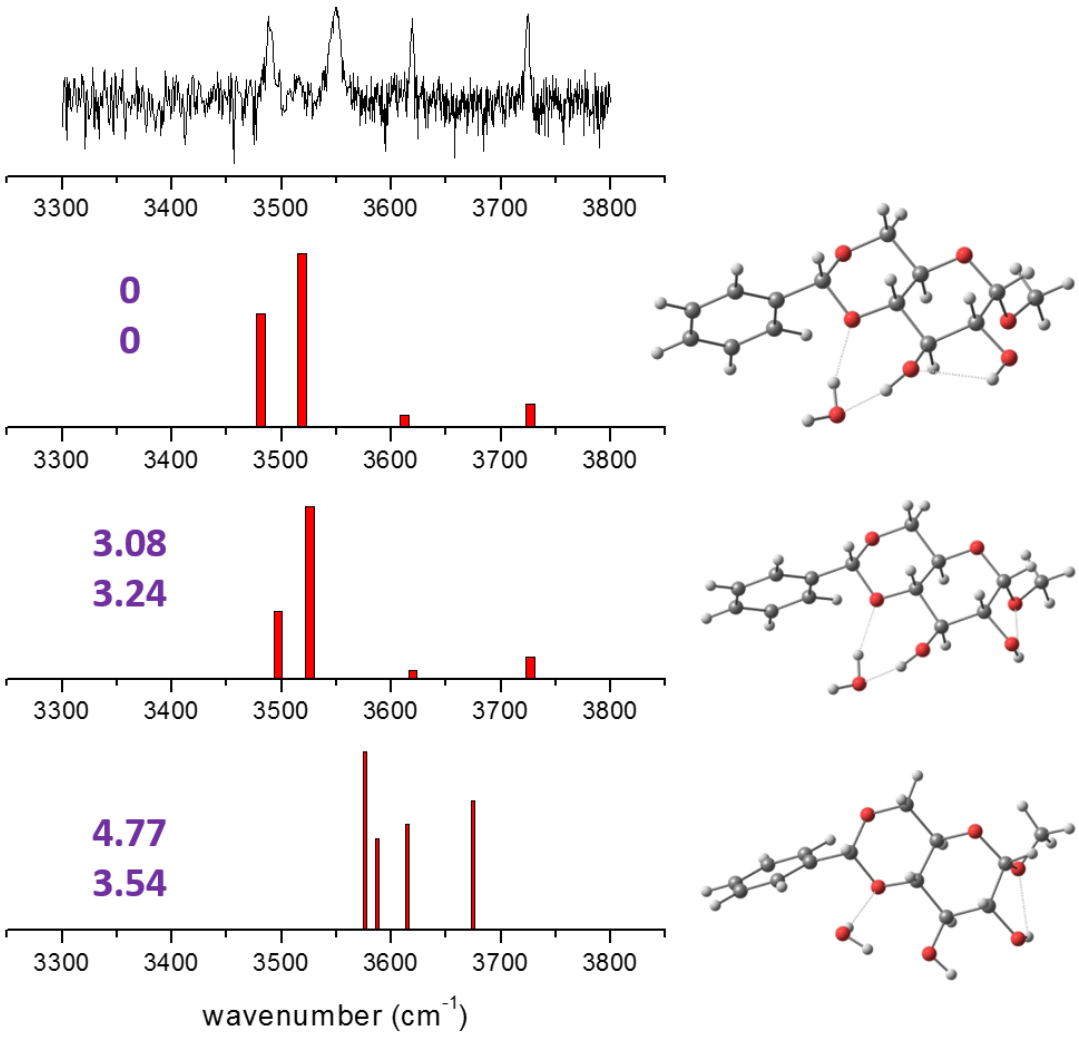

Figure S2-b. Calculated spectra and structure of the most stable conformers of BzGlc-W compared to the IRID spectrum, continued. For each conformer, the relative potential energy is given first and the relative 300 K free energy is given below, in KJ/mol.

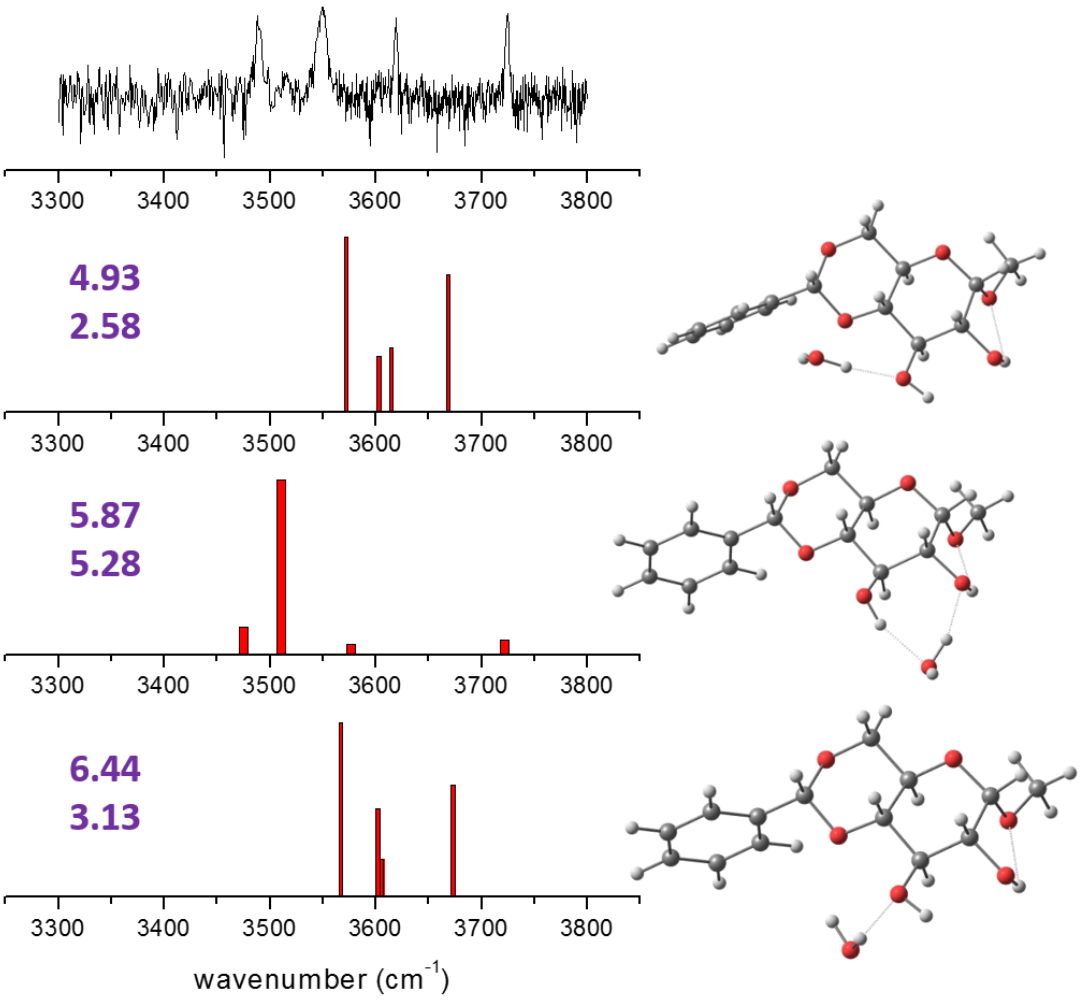

Figure S3-a. Calculated spectra and structure of the most stable conformers of BzGlc-Tol compared to the IRID spectrum. For each conformer, the relative potential energy is given first and the relative 300 K free energy is given below, in KJ/mol.

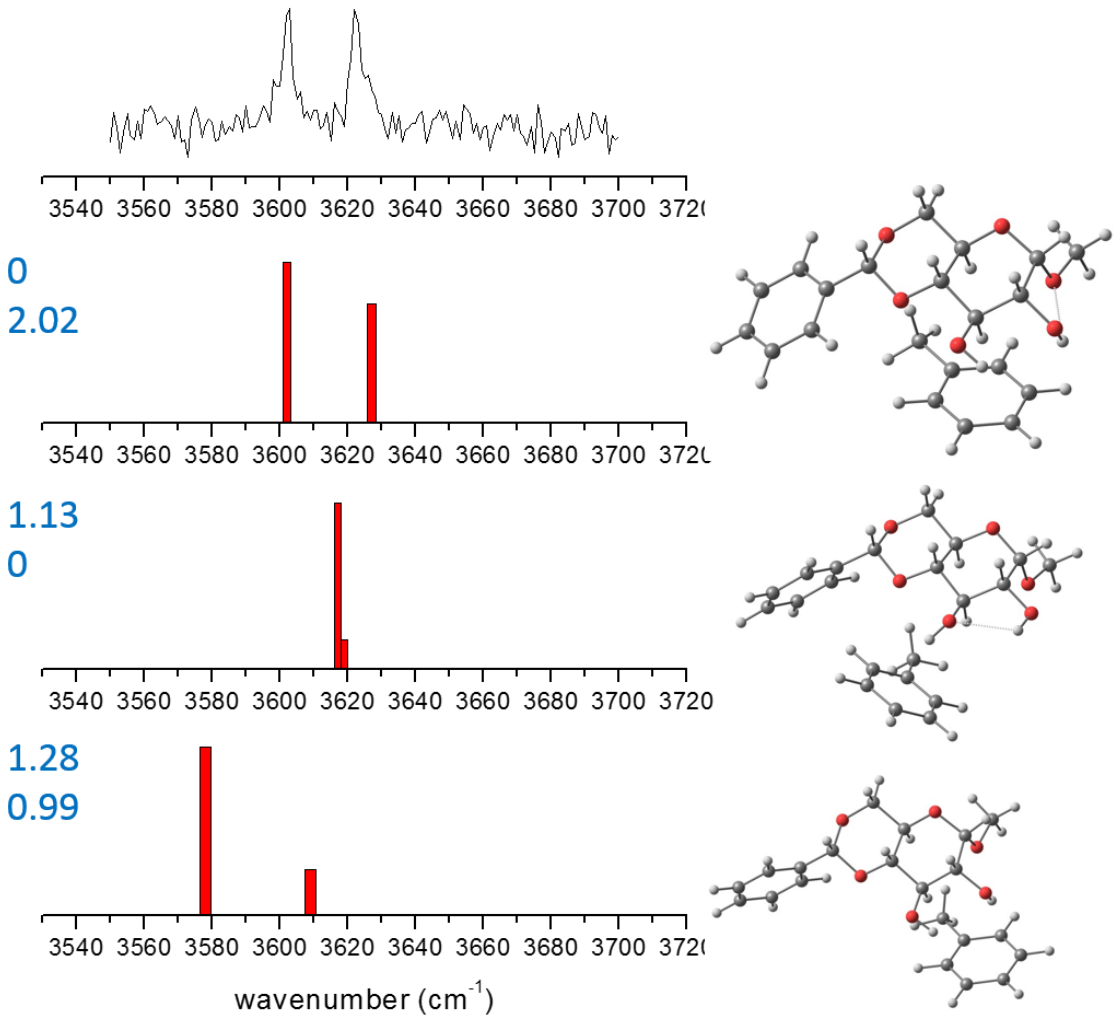

Figure S3-b. Calculated spectra and structure of the most stable conformers of BzGlc-Tol compared to the IRID spectrum, continued. For each conformer, the relative potential energy is given first and the relative 300 K free energy is given below, in KJ/mol.

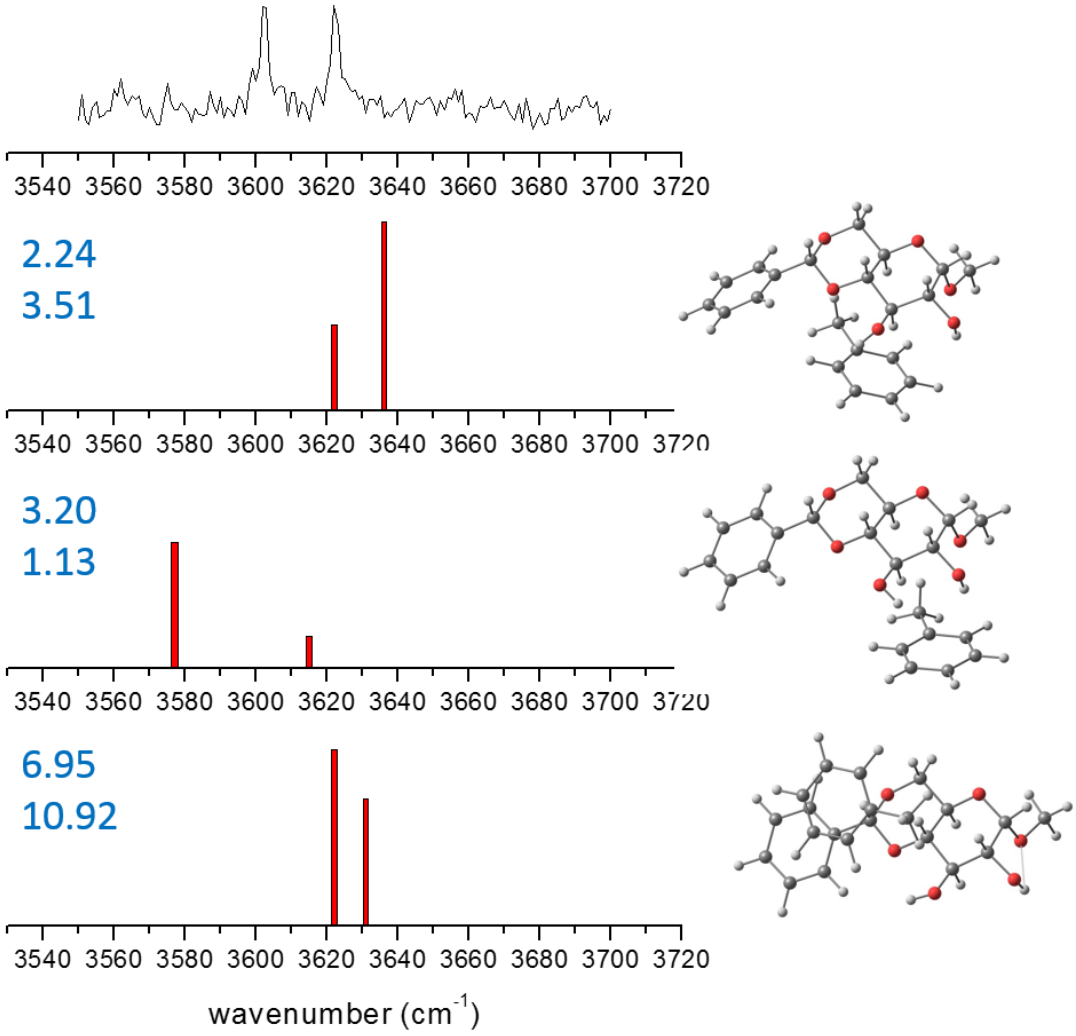

Figure S4-a. Calculated spectra and structure of the most stable conformers of $(BzGlc)_2$ compared to the IRID spectrum. For each conformer, the relative potential energy is given first and the relative 300 K free energy is given below, in KJ/mol.

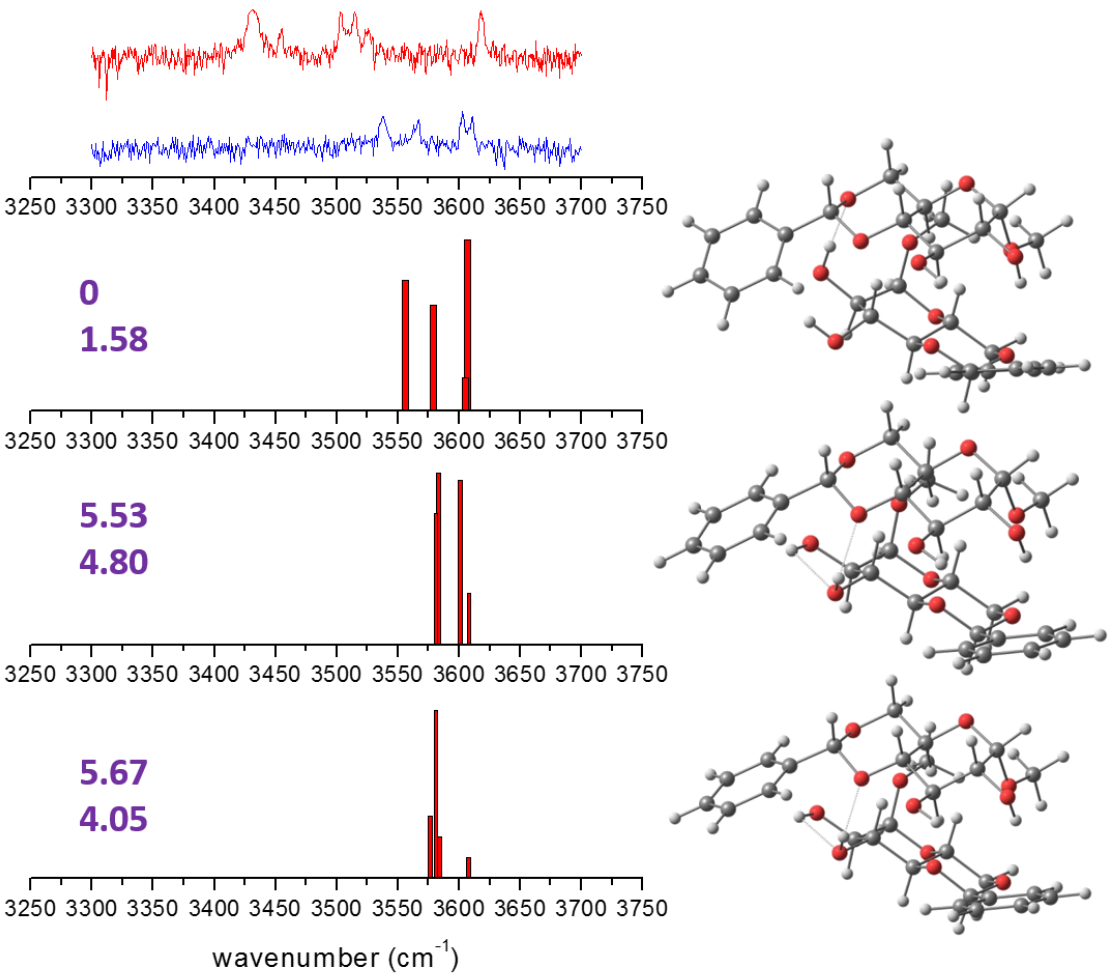

Figure S4-b. Calculated spectra and structure of the most stable conformers of $(BzGlc)_2$ compared to the IRID spectrum, continued. For each conformer, the relative potential energy is given first and the relative 300 K free energy is given below, in KJ/mol.