Supplementary Material

Infrared diagnostic of the conformational change of methylated β-glucose bound to Li^+ upon ligand addition

Oscar Alba Hernandez, Vincent Steinmetz, and Philippe Maître

Université Paris-Saclay, CNRS, UMR8000, Institut de Chimie Physique, 91405, Orsay, France.
Email: philippe.maitre@universite-paris-saclay.fr

Table of Contents

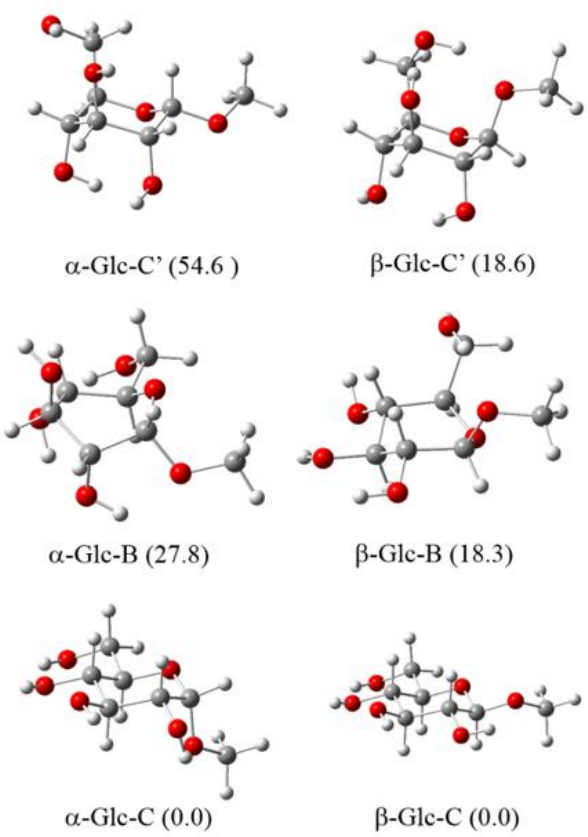

Figure S1. Structure and relative energies (kJ/mol) of the lowest energy structure associated with a chair ($^4C_1$ or $^1C_4$) and one boat configuration for the two methylated monosaccharides. The C, C', and B symbols in the structure names refer to the $^4C_1$, $^1C_4$, and Boat conformers respectively. 298K Gibbs free energies were determined at the B3LYP/6-31G** level of theory.

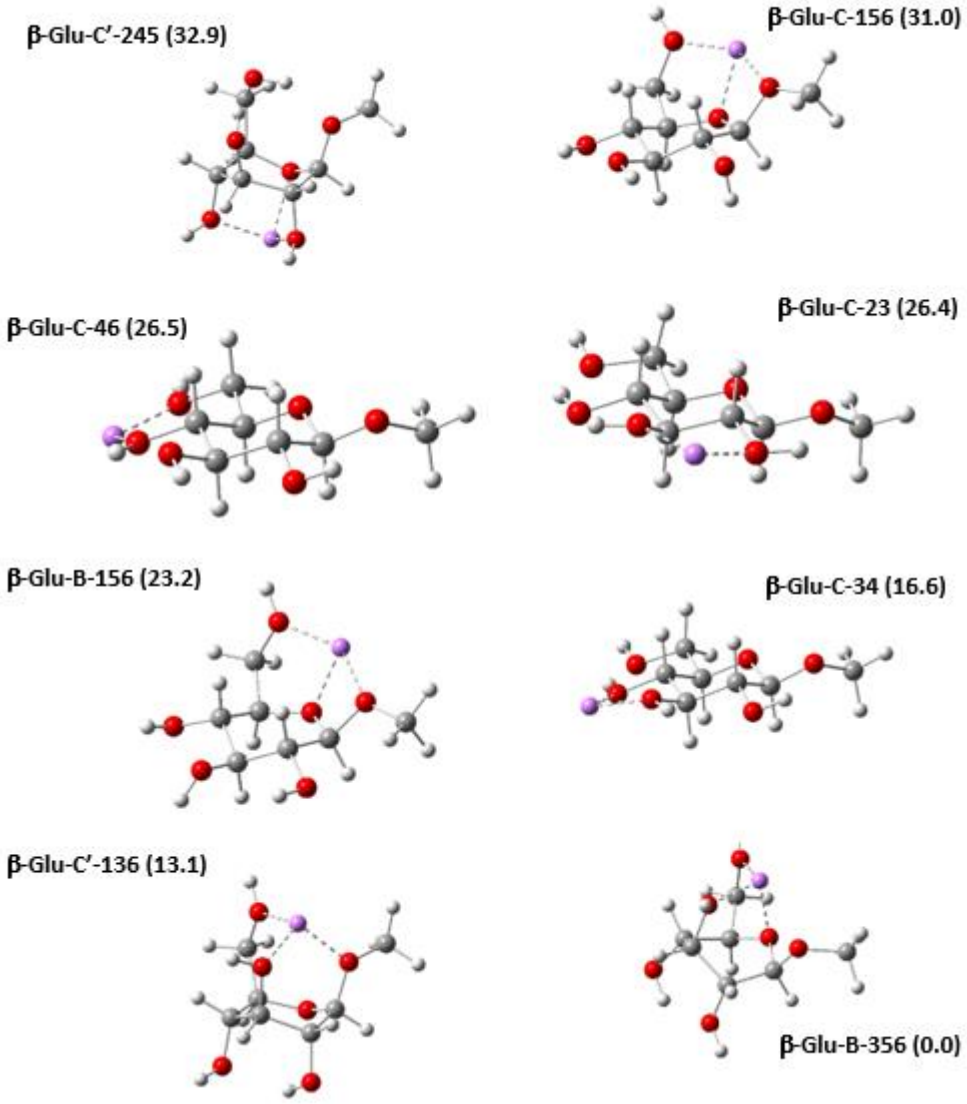

Figure S2. Relative free Gibbs energies of representative structures of the Li(β-Me-Glc)$^+$ complex. Three types of structures are considered, depending on the conformation of the sugar moiety: $^4C_1$, $^1C_4$ and boat conformers are denoted as C, C' and B, respectively. Structures were characterized at the B3LYP/6-31G** level of theory. 298K Gibbs free energies in kJ mol^{-1} are given.

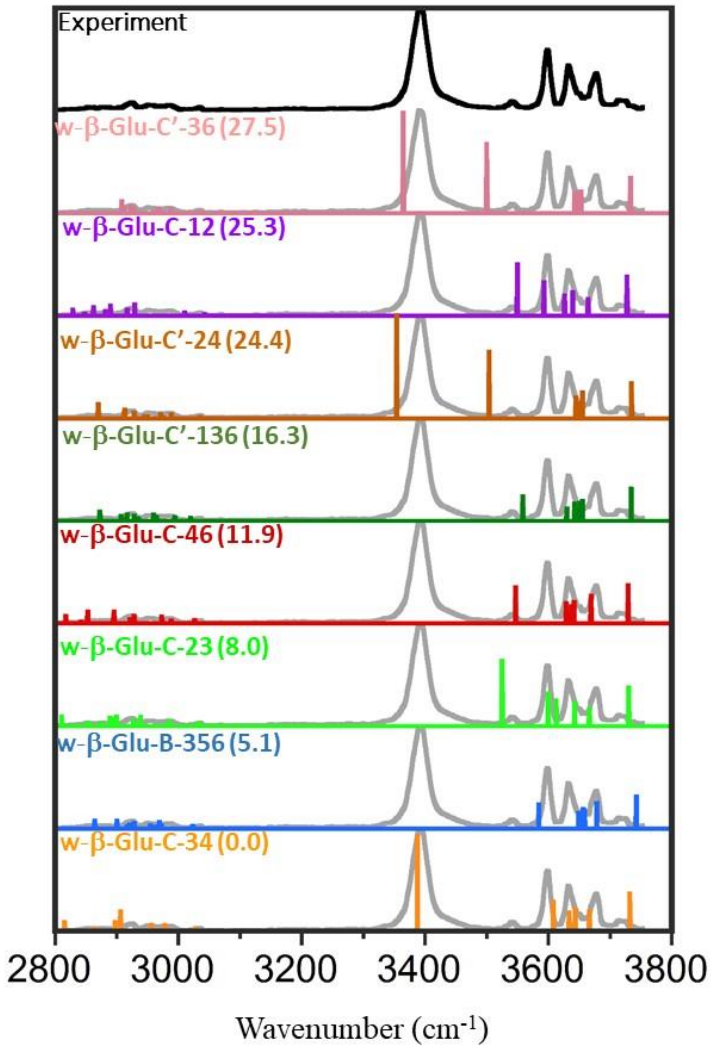

Figure S3. IRMPD spectrum of the Li(β-Me-Glc)$^+$ complex (upper panel). In each of the lower panels, the experimental IRMPD spectrum (grey) is given along with the calculated IR absorption spectrum (stick bars in colour). The relative Gibbs free energies (in kJ mol^{-1}) are also provided. Theoretical infrared absorption spectra were calculated at the B3LYP/6-31G** level of theory, and each band was convoluted using a Gaussian profile with a fwhm of 20 cm^{-1}. Harmonic frequencies were scaled with a factor of 0.955.

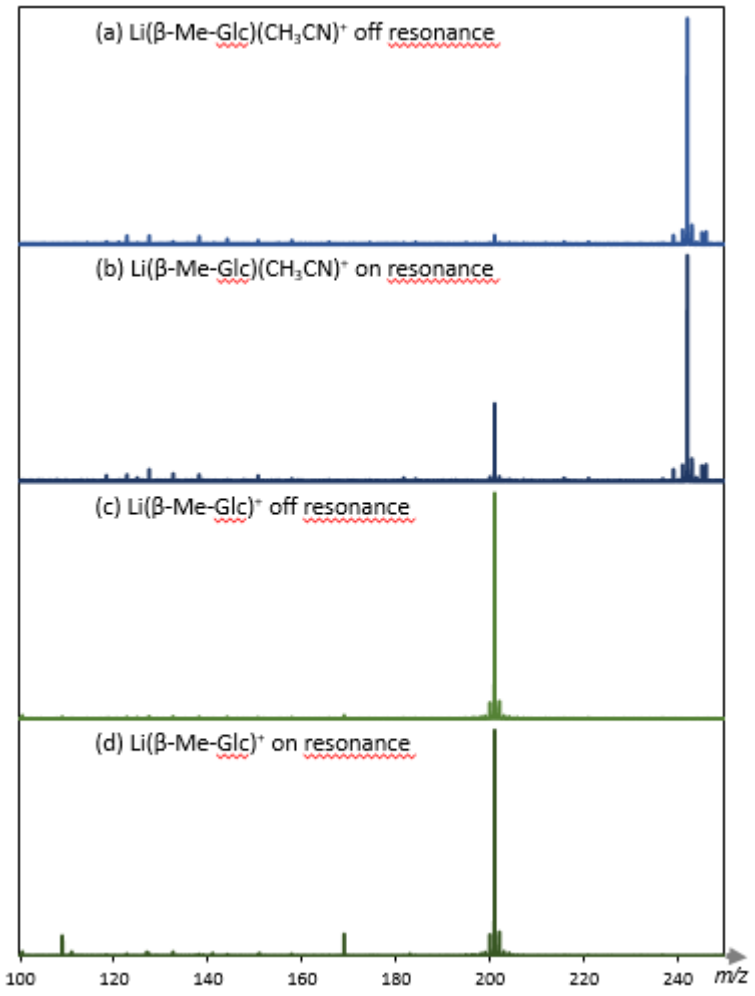

Figure S4. Mass spectra recorded recorded after IR irradiation of the parent ions in the ICR cell. (a) Li(β-Me-Glc)$(CH_3CN)^+$ complex with laser off-resonance; (b) Li(β-Me-Glc)$(CH_3CN)^+$ complex with laser on-resonance evidenced by the m/z 242→201 transition associated with the loss of acetonitrile; (c) Li(β-Me-Glc)$^+$ complex with laser off-resonance; (d) Li(β-Me-Glc)$^+$ complex with laser on-resonance evidenced by the m/z 201→169 transition associated with the loss of methanol.