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

Supporting information

Conformational preferences of the flexible galactofuranose sugar in gas-phase

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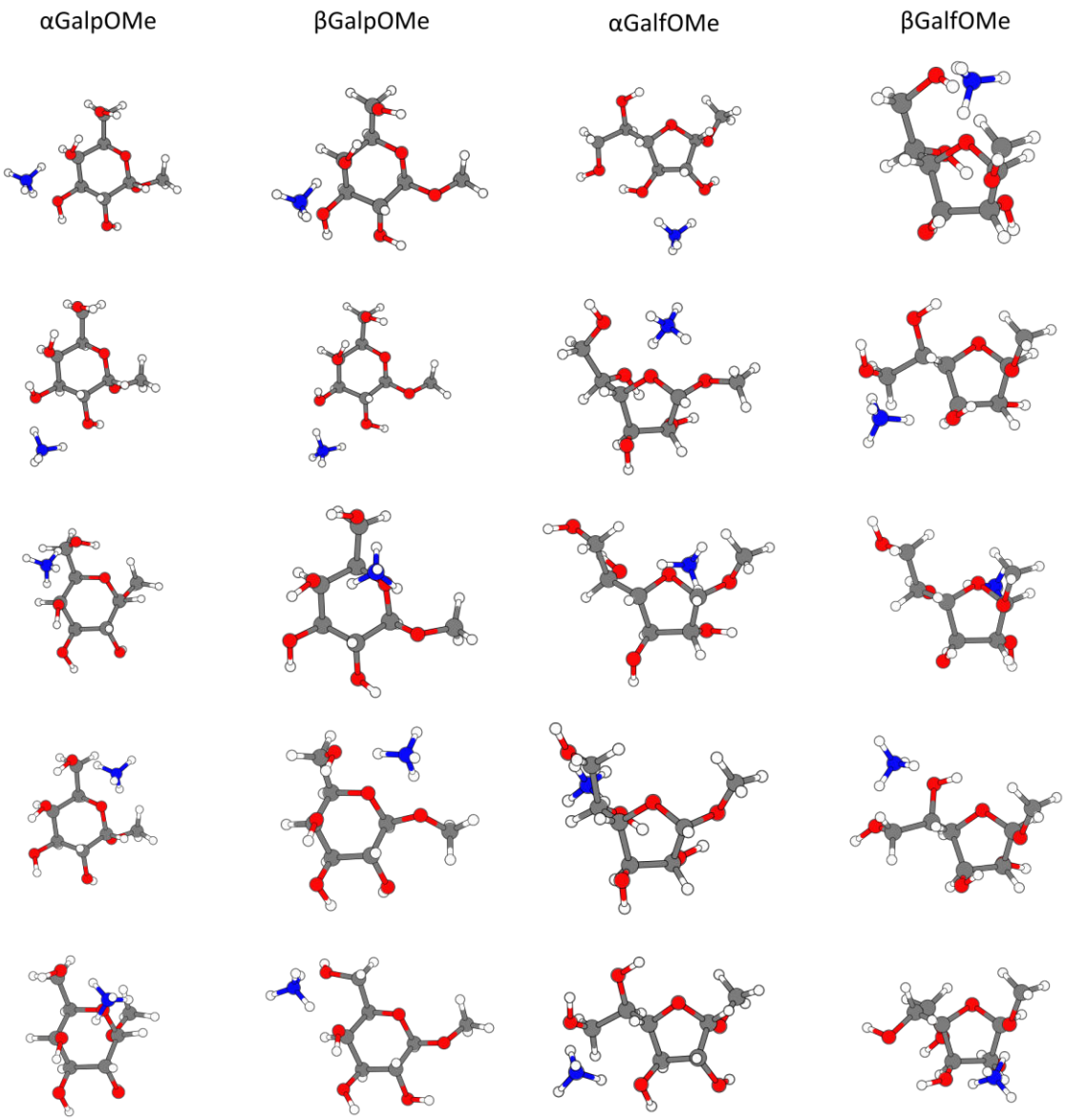


Figure S1 Examples of conformers of αGalpOMe, βGalpOMe, αGalfOMe and βGalfOMe with different NH_4^+ position.

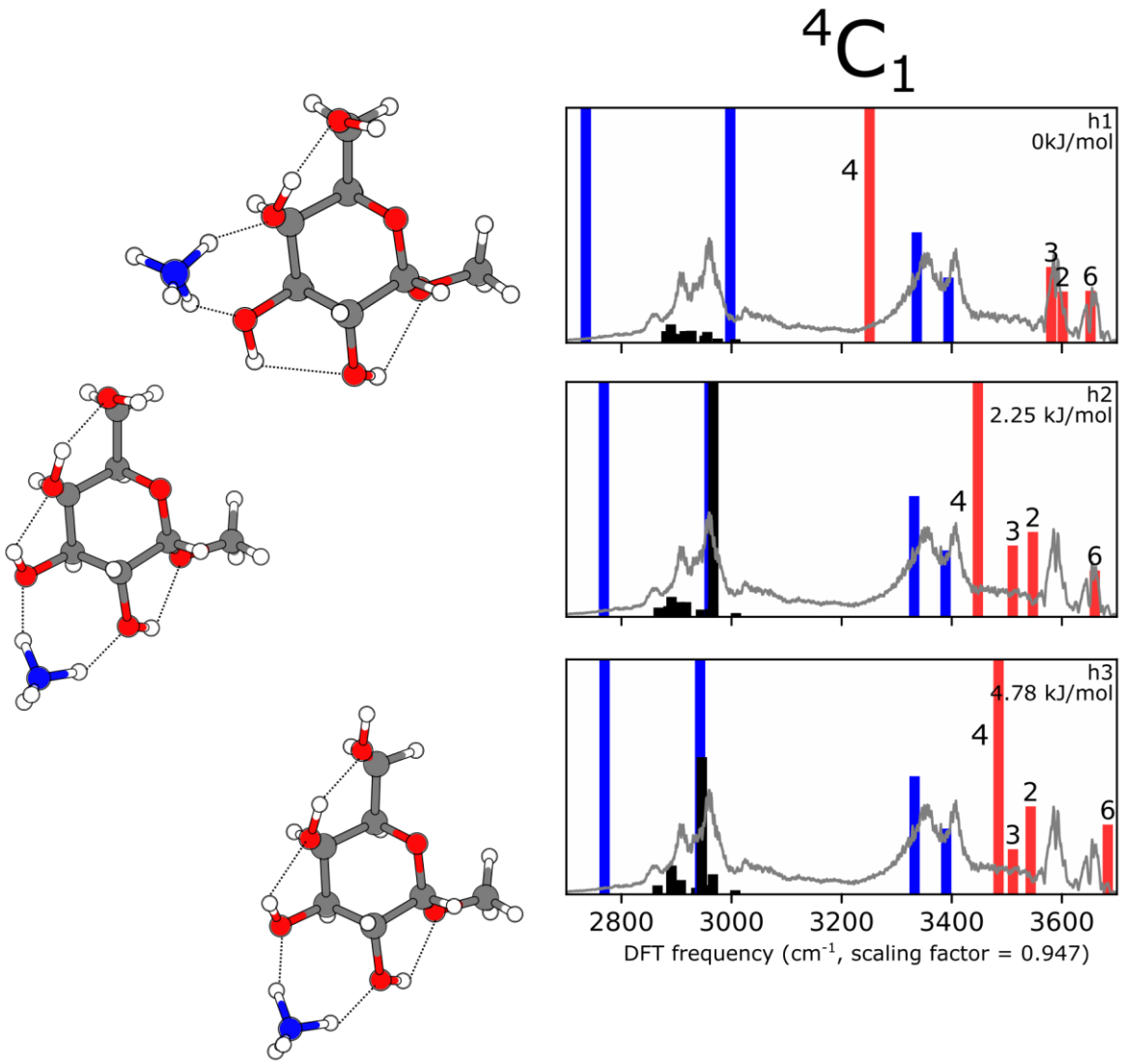


Figure S2 Structures of the most stable conformations for αGalpOMe and their OH (red), NH (blue) and CH (black) vibrational modes compared to the experimental spectrum (grey). The labels indicate the ring OH position. The relative energies are given in reference to the most stable form h1 (only conformers with relative energy under 8.3 kJ/mol are represented). Hydrogen bonds are represented by dotted lines.

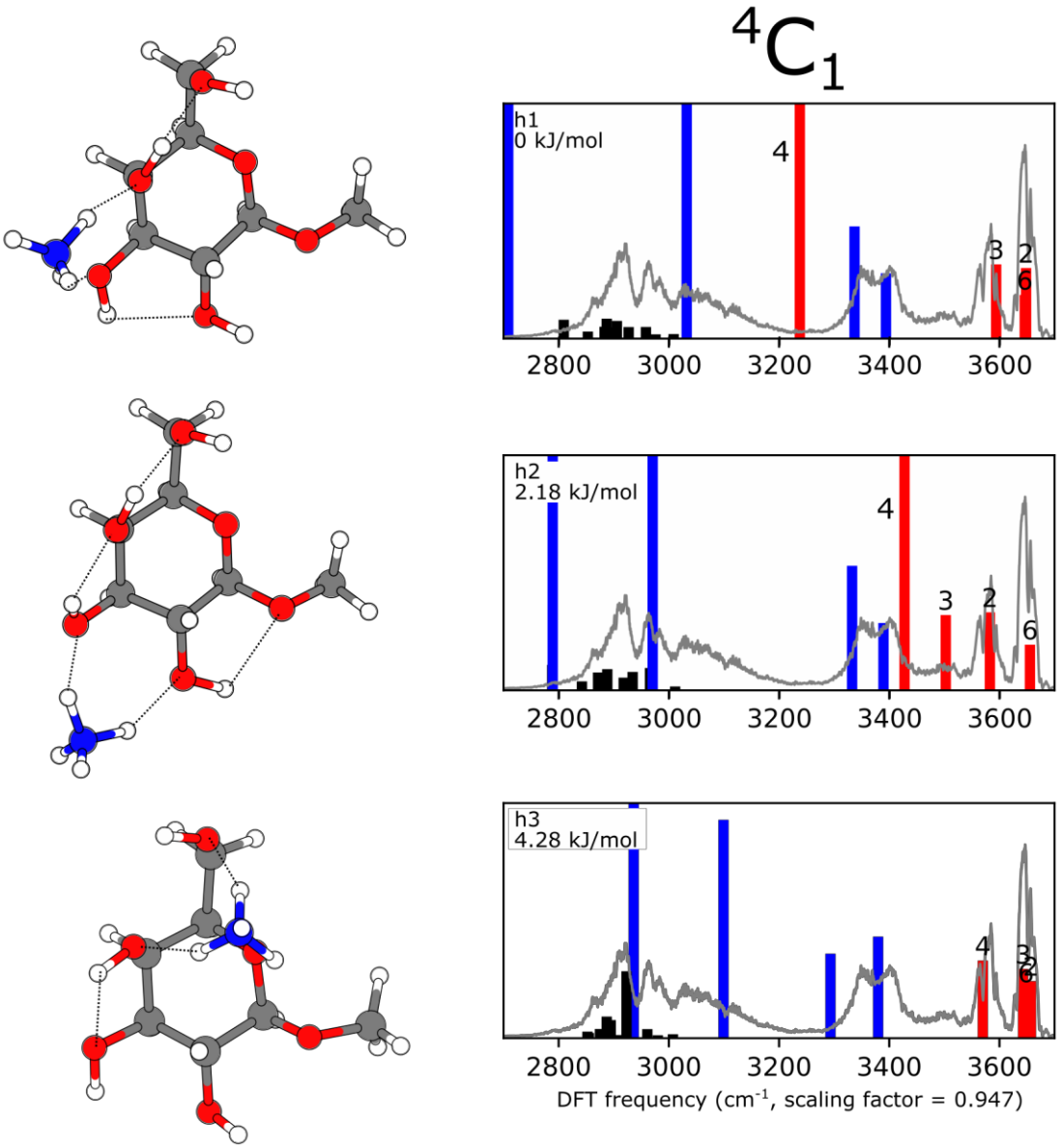
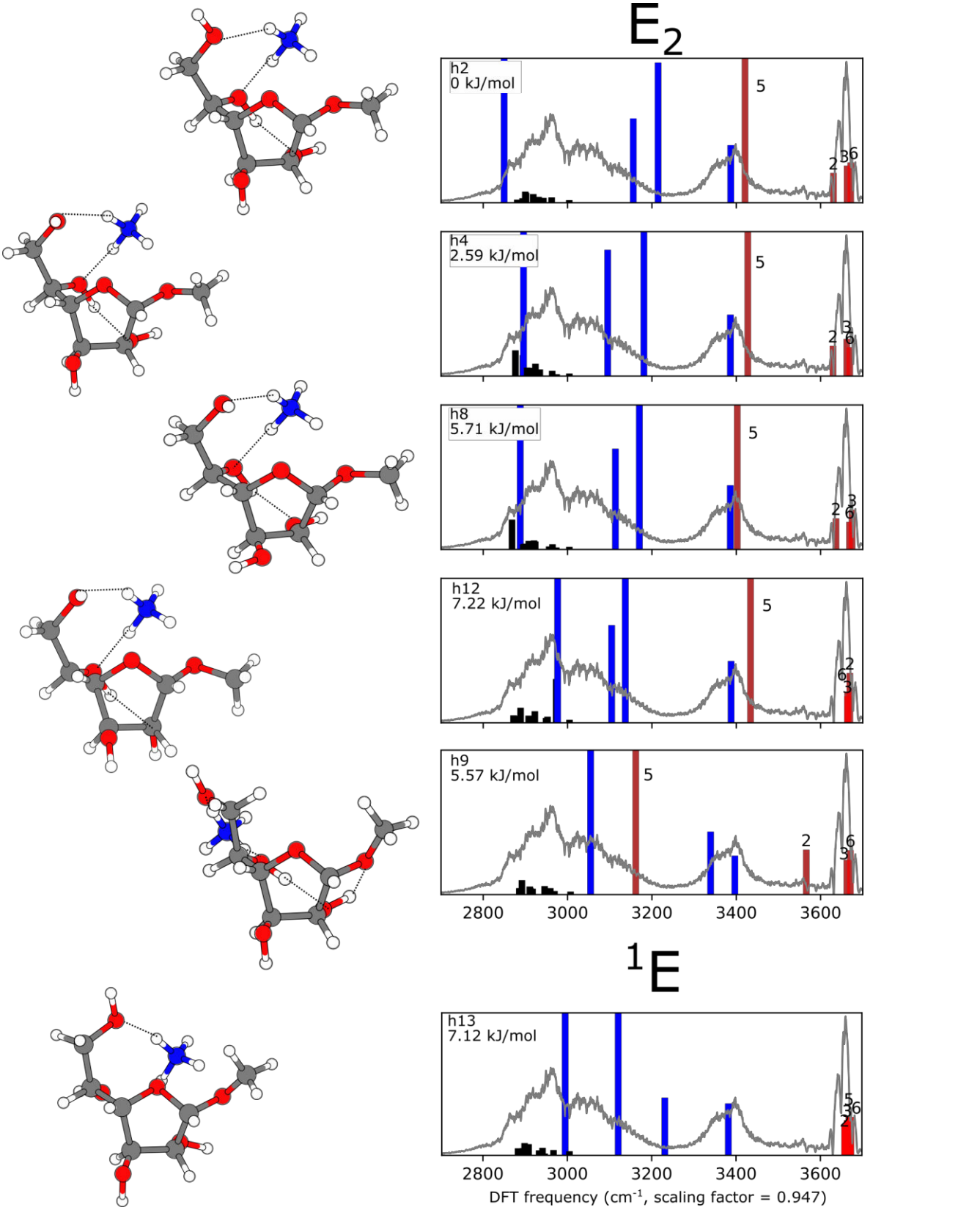


Figure S3 Structures of the most stable conformations for βGalpOMe and their OH (red), NH (blue) and CH (black) vibrational modes compared to the experimental spectrum (grey). The labels indicate the ring OH position. The relative energies are given in reference to the most stable form h1 (only conformers with relative energy under 8.3 kJ/mol are represented). Hydrogen bonds are represented by dotted lines.


E2
h2
0 kJ/mol
h4
2.59 kJ/mol
h8
5.71 kJ/mol
h12
7.22 kJ/mol
h9
5.57 kJ/mol
1E
h13
7.12 kJ/mol
2800
3000
3200
3400
3600
DFT frequency (cm-1, scaling factor = 0.947)

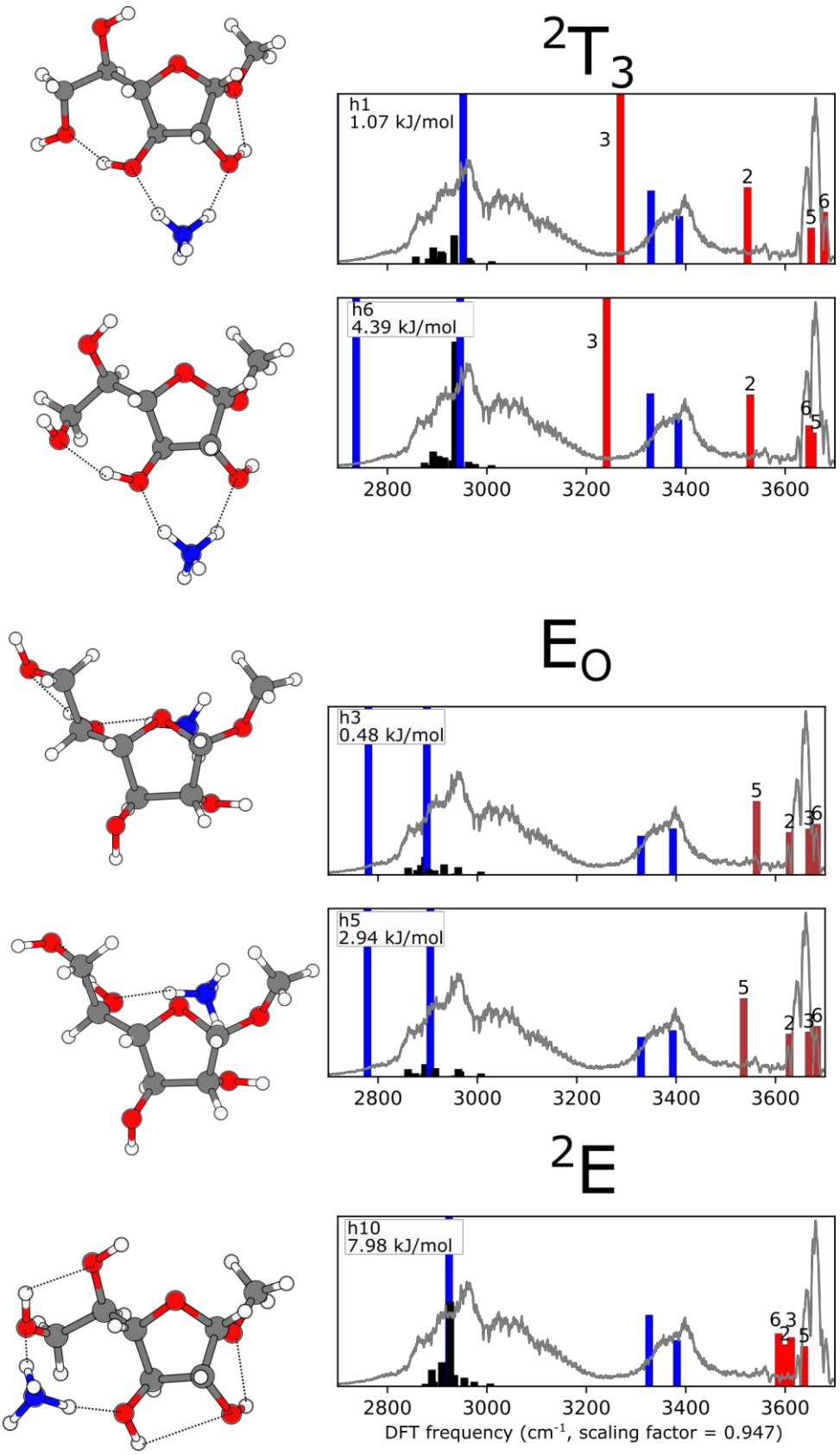
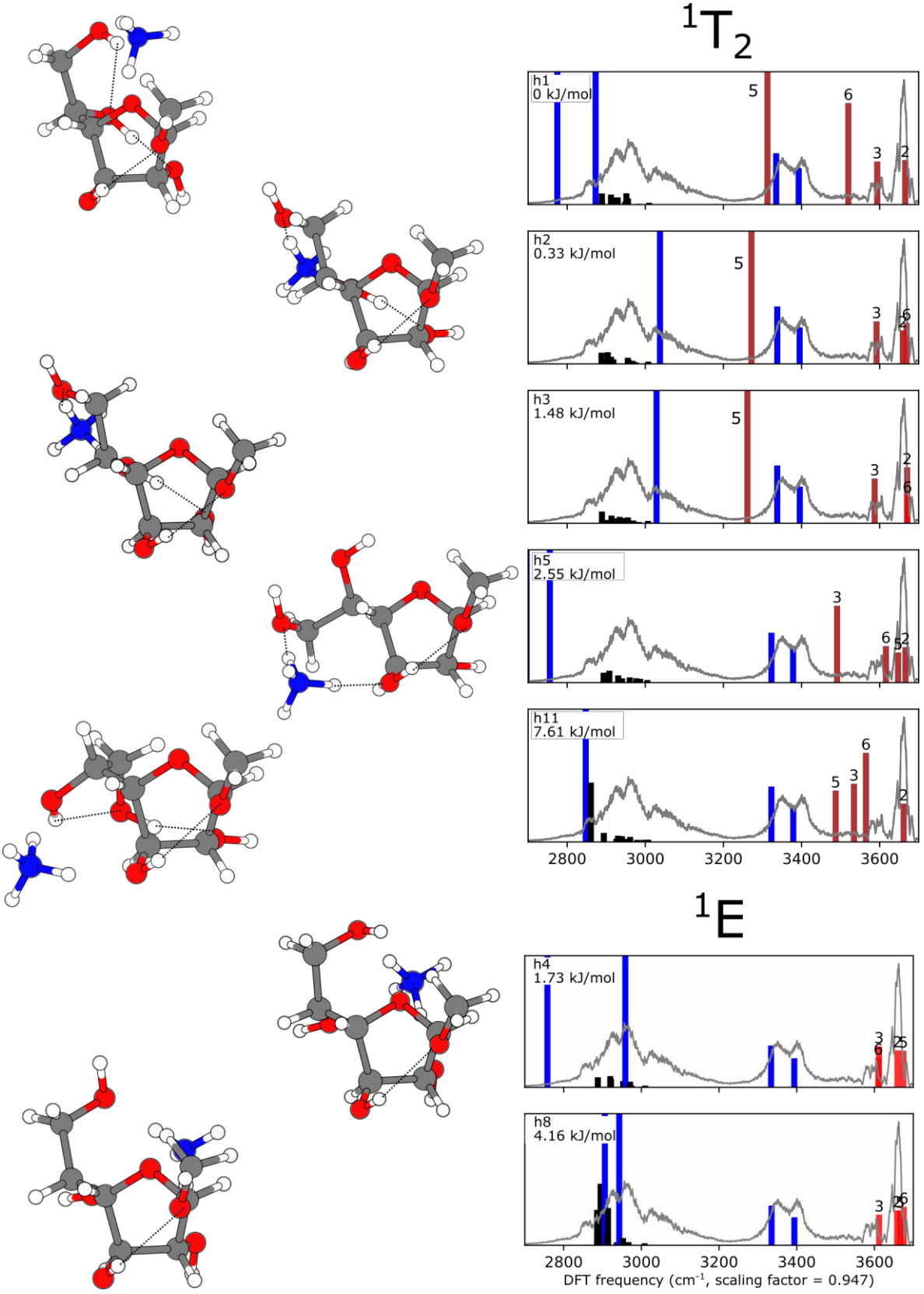


Figure S4 Structures of the most stable conformations for αGalfOMe, gathered according to their geometry type, and their OH (red), NH (blue) and CH (black) vibrational modes compared to the experimental spectrum (grey). The labels indicate the ring OH position. The relative energies are given in reference to the most stable form h1 (only conformers with relative energy under 8.3 kJ/mol are represented). Hydrogen bonds are represented by dotted lines.


$^1T_2$
h1
0 kJ/mol
h2
0.33 kJ/mol
h3
1.48 kJ/mol
h5
2.55 kJ/mol
h11
7.61 kJ/mol
^1E
h4
1.73 kJ/mol
h8
4.16 kJ/mol
2800
3000
3200
3400
3600
DFT frequency (cm^{-1}, scaling factor = 0.947)

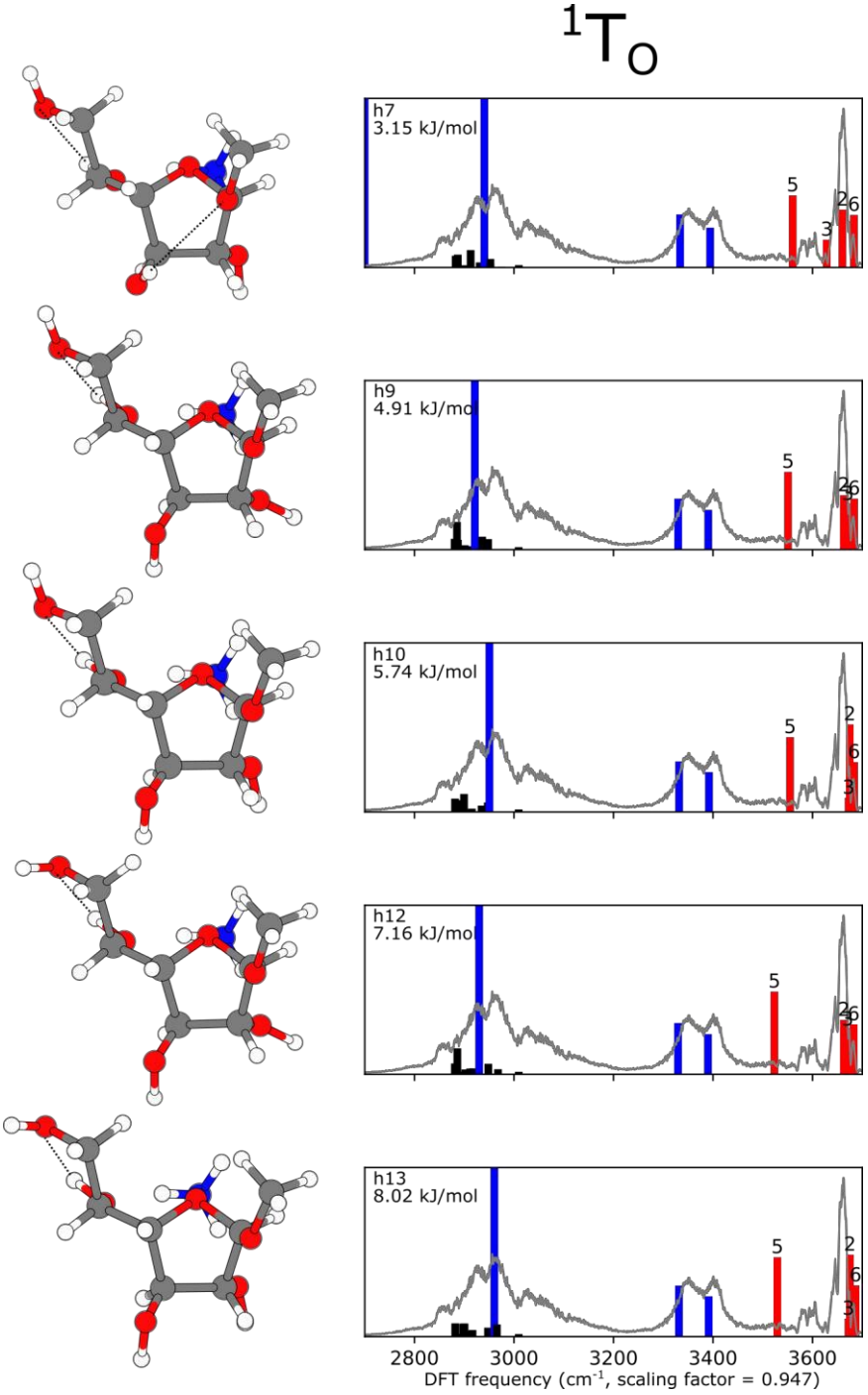


Figure S5 Structures of the most stable conformations for βGalfOMe, gathered according to their geometry type, and their OH (red), NH (blue) and CH (black) vibrational modes compared to the experimental spectrum (grey). The labels indicate the ring OH position. The relative energies are given in reference to the most stable form h1 (only conformers with relative energy under 8.3 kJ/mol are represented). Hydrogen bonds are represented by dotted lines.