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

Hydrogen Bonding and Dominant Conformation of Hydrated Sugar Analogue Complexes: Tetrahydrofurfuryl Alcohol as the Example

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Supporting Information

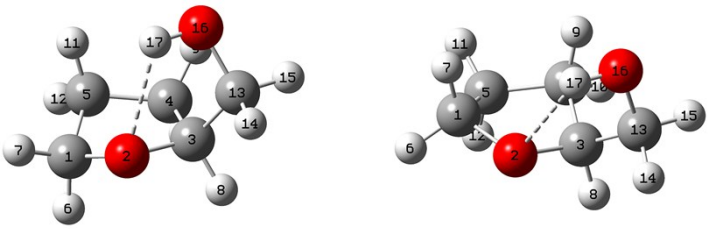

Fig. S1 The most abundant conformer of monomer THFA. The envelope structure is named as Conformer THFA-C, and the twisted structure is named as Conformer THFA-A.

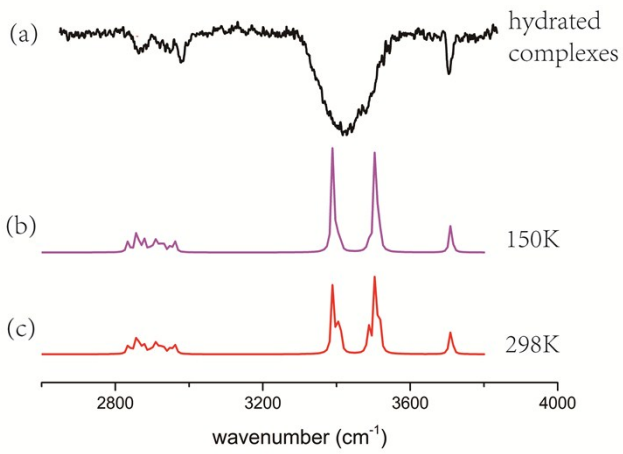

Fig. S2 Computed IR spectra of the most abundant conformer of hydrated THFA complexes at two different temperatures with the experimental results for comparison. A Lorentzian profile with a FWHM of 20 cm^{-1} is used to convolute the calculated spectra.

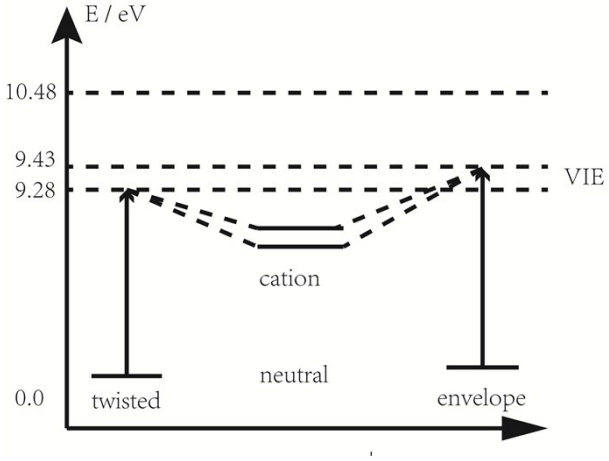

Fig. S3 Energy diagram of the VUV one-photon ionization of hydrated THFA from the neutral ground state. The stable structures and transition states of the cation were searched at mp2/aug-cc-pVTZ level of theory.

Table S1 The parameters of the neutral and cationic hydrated THFA complexes. (pm)

conformer	A-I	A-II	C-I	trans-hc	cis-hc
O2-H19	181.7	184.2	181.2		
C3-C13	140.1	140.3	140.2	130.5	130.1
O16-H17	96.7	96.7	96.7	99.6	99.4
H17-O18	190.6	191.7	190.7	162.2	163.6