STRUCTURAL EXPRESSION OF EXO-ANOMERIC EFFECT

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Structural signatures for exo–anomeric effect have been extracted from the archetypal methyl–β–D–xyloside using broadband Fourier transform microwave spectroscopy combined with laser ablation. Spectrum analysis allows the determination of a set of rotational constants, which has been unequivocally attributed to conformer cc–β-$^4C_1$ g-, corresponding to the global minimum of the potential energy surface, where the aglycon residue (CH_3) orientation contributes towards maximization of the exo-anomeric effect. Further analysis allowed the determination of the r_s structure, based on the detection of eleven isotopologues - derived from the presence of six ^{13}C and five ^{18}O atoms - observed in their natural abundances. The observed glycosidic C_1-O_1 bond length decrease (1.38 Å) can be interpreted in terms of the exo–anomeric effect. As such, the exo–anomeric effect presents itself as one of the main driving forces controlling the shape of many biologically important oligosaccharides.