Computational insights into octyl-*D*-xyloside isomers toward understanding the liquid crystalline structure: physico-chemical features

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Supplementary Information

Table S1 Calculated properties of xyloside isomers in gas phase, including dipole moment μ (Debye), Gibbs and relative free energy (kcal.mol⁻¹), H bonds (HB) and O–H bonds lengths as well as dihedral angles between OH groups involved in HB (all at B3LYP/6-31+G(d,p))

Molecule	μ (D) Calculated G Relative G	HB (O _x H _x –O _y)	O _x –H _x (Å)	H _x –O _y (Å)	Dihedral angle O _x –C _x –C _y –O _y (°)
1a	2.89	O ₄ H···O ₃	2.44	0.968	-63.76
	-556528.45	O ₃ H···O ₂	2.50	0.968	62.82
	0.00	O ₂ H···O ₁	2.22	0.970	51.56
1b	1.53	O ₃ H···O ₄	2.52	0.967	-65.86
	-556525.02	O ₂ H···O ₃	2.38	0.968	61.75
	3.43				
2a	2.69	O ₄ H···O ₃	2.46	0.968	-65.19
	-556528.13	O ₃ H···O ₂	2.48	0.968	64.68
	0.33	O ₂ H···O ₁	2.50	0.968	-64.31
2b	3.07	O ₃ H···O ₄	2.49	0.968	58.10
	-556524.71	O ₂ H···O ₃	2.40	0.968	-52.10
	3.74				
3	3.59	O ₅ H···O ₃	2.10	0.969	-44.00
	-556525.22	O ₂ H···O ₁	2.16	0.971	40.27
	3.23				
4	3.80	O ₅ H···O ₃	2.10	0.969	-33.14
	-556522.92				
	5.53				
5	4.03	O ₄ H···O ₂	1.89	0.973	34.88
	-556523.43	O ₂ H···O ₁	2.23	0.969	-56.84
	5.02				