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_xH_x–O_y)	Ox–Hx (Å)	H_x–O_y (Å)	Dihedral angle O_x–C_x–C_y–O_y (°)
1a	2.89 -556528.45 0.00	$O_4H\cdots O_3$ $O_3H\cdots O_2$ $O_2H\cdots O_1$	2.44 2.50 2.22	0.968 0.968 0.970	-63.76 62.82 51.56
1b	1.53 -556525.02 3.43	$O_3H\cdots O_4$ $O_2H\cdots O_3$	2.52 2.38	0.967 0.968	-65.86 61.75
2a	2.69 -556528.13 0.33	$O_4H\cdots O_3$ $O_3H\cdots O_2$ $O_2H\cdots O_1$	2.46 2.48 2.50	0.968 0.968 0.968	-65.19 64.68 -64.31
2b	3.07 -556524.71 3.74	$O_3H\cdots O_4$ $O_2H\cdots O_3$	2.49 2.40	0.968 0.968	58.10 -52.10
3	3.59 -556525.22 3.23	$O_5H\cdots O_3$ $O_2H\cdots O_1$	2.10 2.16	0.969 0.971	-44.00 40.27
4	3.80 -556522.92 5.53	$O_5H\cdots O_3$	2.10	0.969	-33.14
5	4.03 -556523.43 5.02	$O_4H\cdots O_2$ $O_2H\cdots O_1$	1.89 2.23	0.973 0.969	34.88 -56.84