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Interaction and Reaction of Hydroxyl Ion with β-D-Galactose and its Hydrated Complex: An Ab Initio Molecular Dynamics Study

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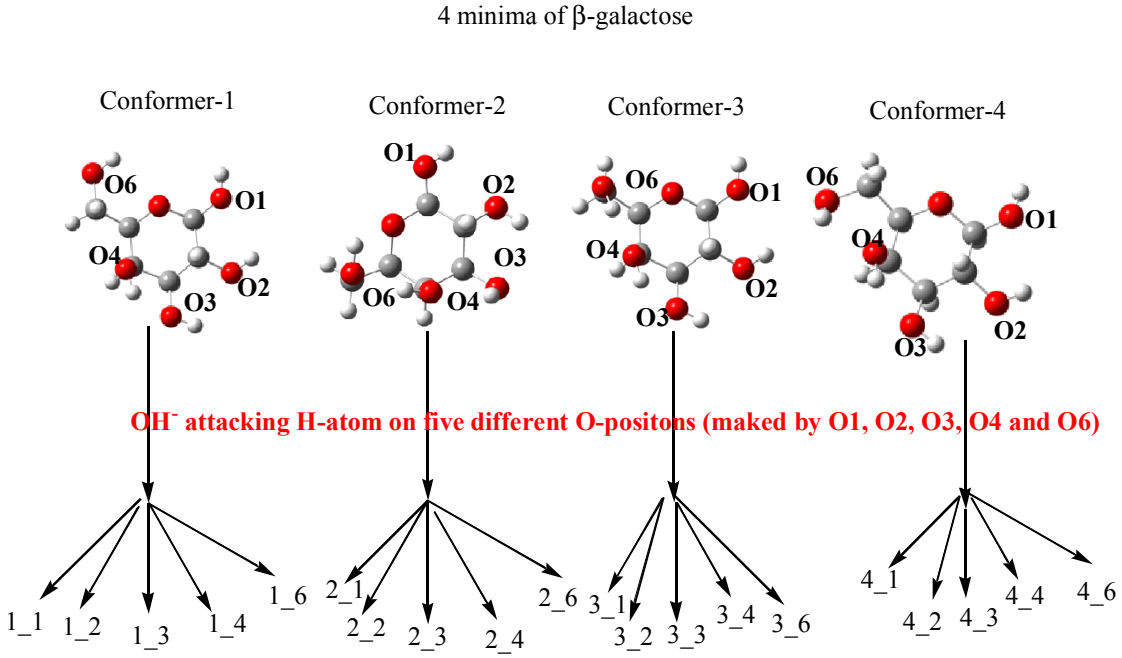
Supporting Information:

S1: Details for searching for global minimum of β-D-galactose+OH^-

We took the minima (four structures with lower energy) of β-D-galactose from recent reference[1] as the initial structures. According to scheme 1, 20 initial structures were built for β-D-galactose +OH^- using the four β-D-galactose minima. Then, they were optimized at BLYP-D/def2-TZVP and SOS-RIMP2/def2-TZVP level with Turbomole[2] package. All optimizations lead to Deprotonated β-D-Galacose anion **(Dep-beta-D-G)**$^-$+H_2O. The energy information is presented in Table S1.



The names of 20 initial structures of Beta-galactose+OH^-

Scheme S1: The scheme to build initial structures of β-D-galactose+OH^-

Table S1: Relative energy (kcal/mol) of 20 conformers at BLYP-D/def2-TZVP and SOS-RIMP2/def2-TZVP () level, respectivrly.

Isomer	Relative energy	Isomer	Relative energy
1_1	2.8 (2.6)	3_1	4.4 (5.6)
1_2	11.8 (10.8)	3_2	12.0 (11.6)
1_3	11.9 (11.1)	3_3	9.9 (9.4)
1_4	19.4 (18.8)	3_4	8.7 (9.4)
1_6	22.5 (22.7)	3_6	28.9 (30.6)
2_1	4.4 (10.0)	4_1	3.8 (4.4)
2_2	8.8 (10.1)	4_2	12.4 (11.5)
2_3	13.2 (14.2)	4_3	10.7 (10.0)
2_4	0.0 (0.0)	4_4	8.7 (9.4)
2_6	1.7 (2.0)	4_6	21.9 (22.4)

S2: Computational details for dynamics of β-galactose+OH^-

Density function theory (DFT) with the BLYP functional along with a triple-ξ valence polarized basis set (TZVP) within the resolution-of-the-identity (RI)[3] approximation was used to conduct Ab Initio Molecular Dynamics calculations. A general drawback of most standard DFT methods is that they do not describe van der Waals (vdW, dispersive) forces[4]. The dispersion correction introduced by S. Grimme[5] for the BLYP functional is adopted, since van der Waals interactions may play a role in the system studied. We used Nosé-Hoover thermostat[6,7] to keep temperature of the system. One time step was 0.5 fs. The total length of each Ab Initio Molecular Dynamics (AIMD) simulation was 10 ps. Calculations were conducted using TURBOMOLE[2] package. For the systems we run multiple trajectories, particle momenta were sampled from the Maxwell distribution at the inverse temperature.

S3: Videos describing the trajectoris of the simulations

The reperesentative trajectories for β-D-galactose $+OH^-+(H_2O)n$(n=0,1 and 2) are attached. In the process of making videos, we save one snapshot in every 5 fs.

Reference:

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4. Grimme, S. J. Comput. Chem. 2006, 27, 1787.
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