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

Supplementary material

Collision-Induced Dissociation of Sodiated Glucose and Identification of Anomeric Configuration

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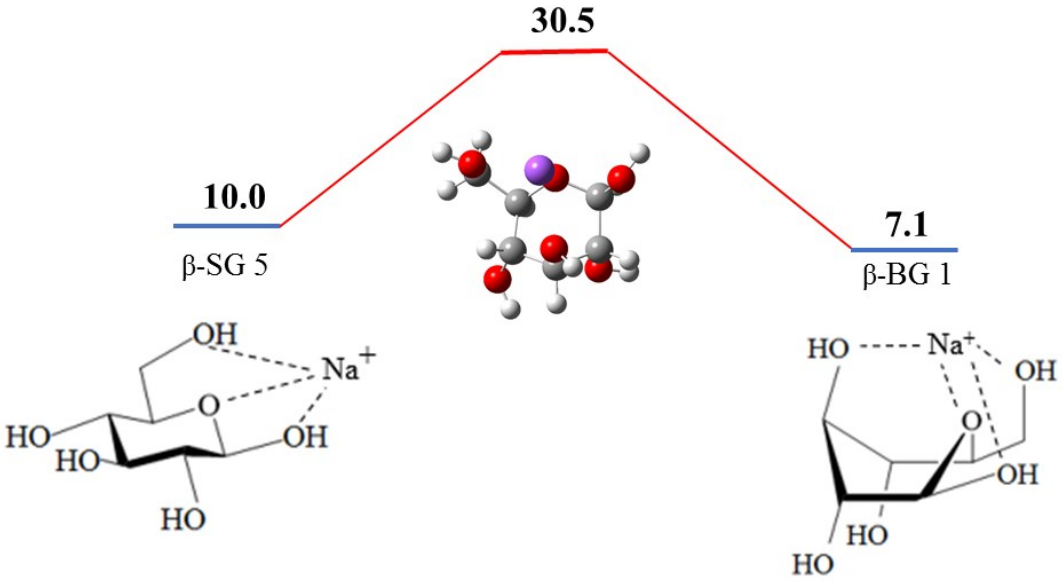


Figure S1. The barrier (kJ/mol) for the change from sodiated β-glucose of chair conformation to sodiated β-glucose of boat conformation. The zero potential energy is set at the most stable conformer of sodiated α-glucose (β-SG3, see Figure S2).B3LYP functional with the 6-311+G(d,p) basis set was used in calculations.

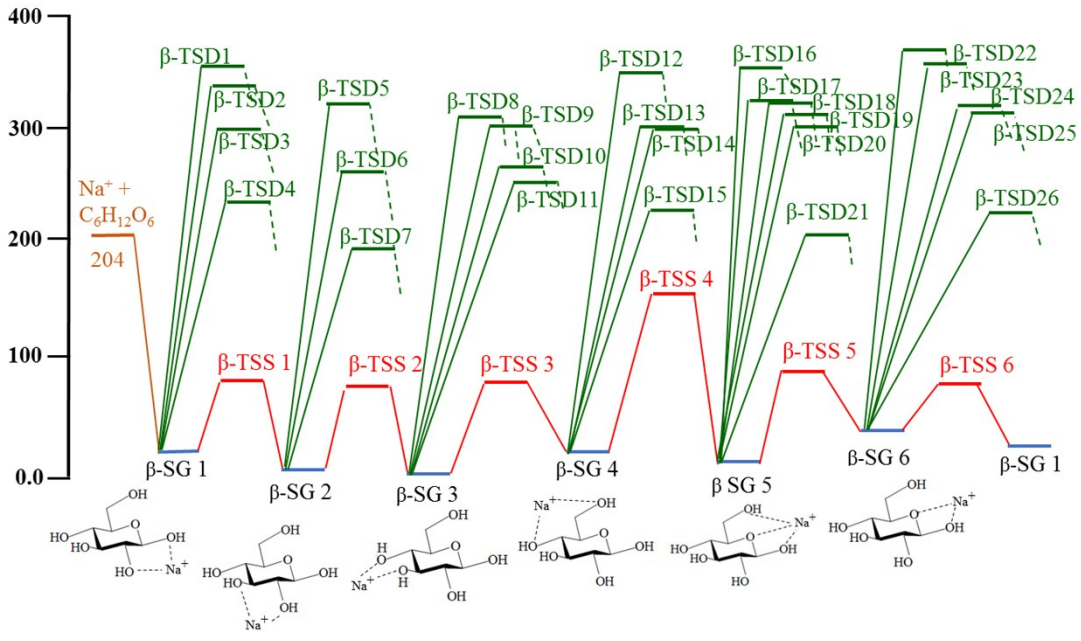


Figure S2. Geometries and relative energies (kJ/mol) of sodiated β-glucose with chair

conformation $^{4}C_{1}$ (blue lines), sodium cation migration barriers (red lines), and dehydration reaction barriers (green lines). The energy levels of dehydration products are not shown. The zero potential energy is set at the most stable conformer β-SG3. B3LYP functional with the 6-311+G(d,p) basis set was used in calculations.

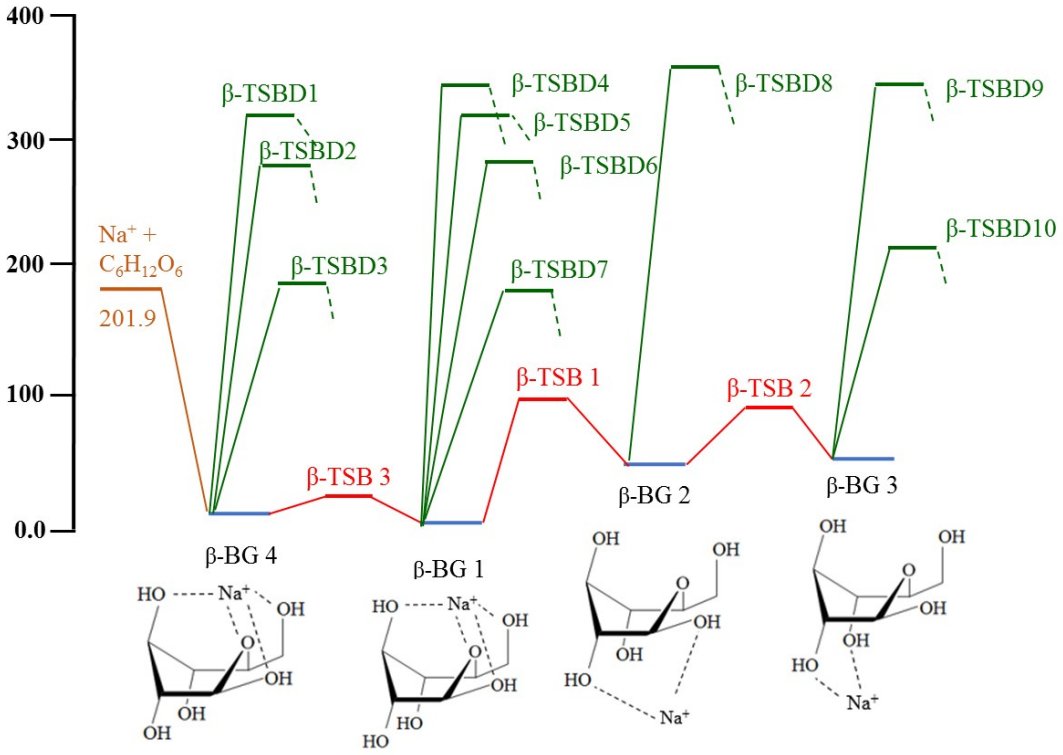
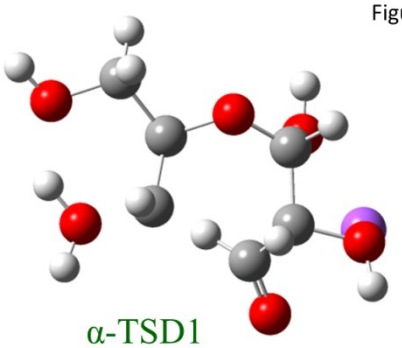


Figure S3. Geometries and relative energies (kJ/mol) of sodiated β-glucose with boat conformation $^{0,3}B$ (blue lines), sodium cation migration barriers (red lines), and dehydration reaction barriers (green lines). The energy levels of dehydration products are not shown. The zero potential energy is set at the most stable conformer β-SG3. B3LYP functional with the 6-311+G(d,p) basis set was used in calculations.

Figure S4-1



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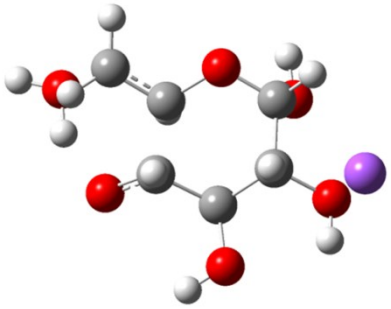

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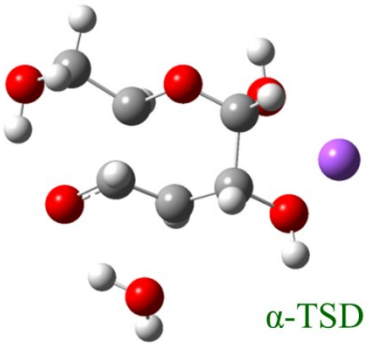

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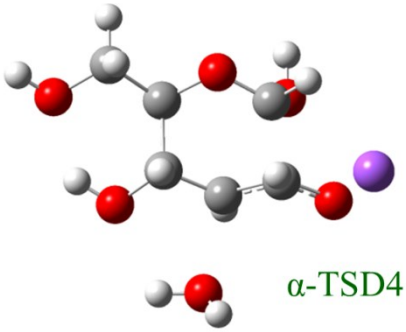

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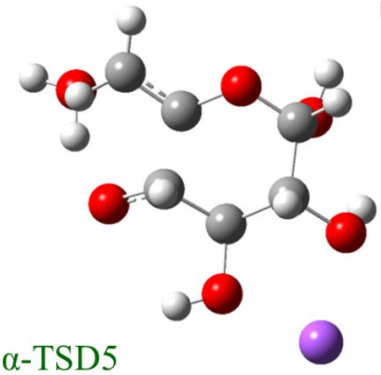
Figure S4-2



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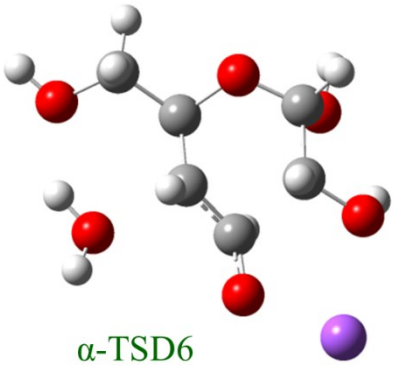

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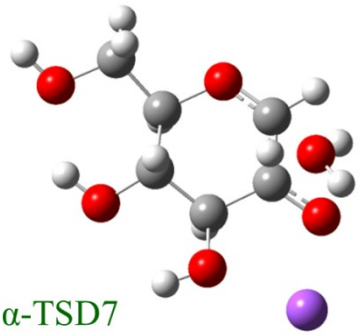

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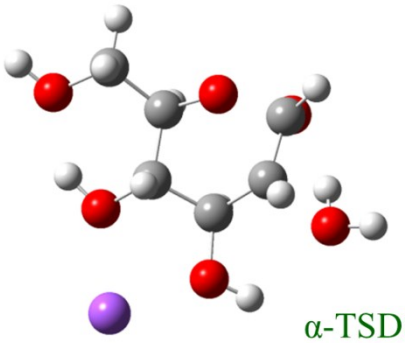

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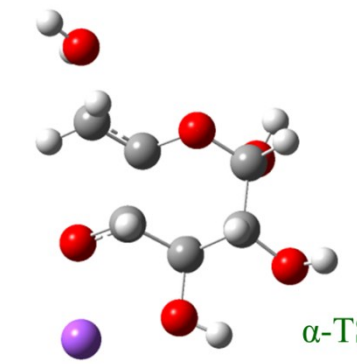

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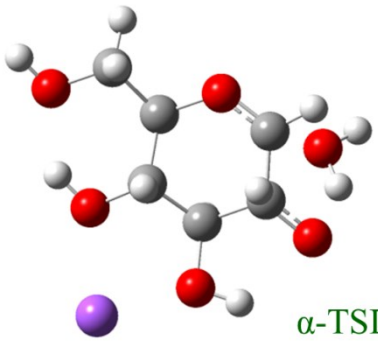

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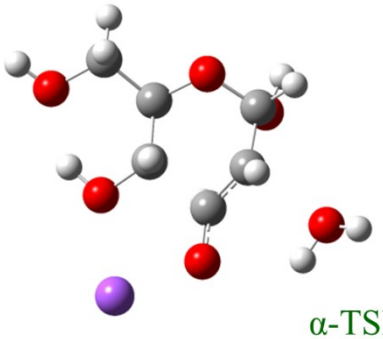

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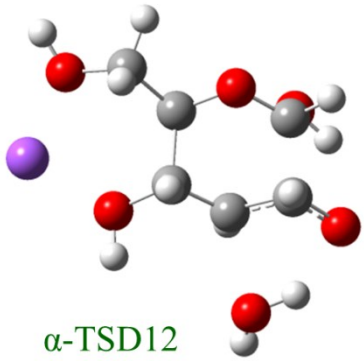

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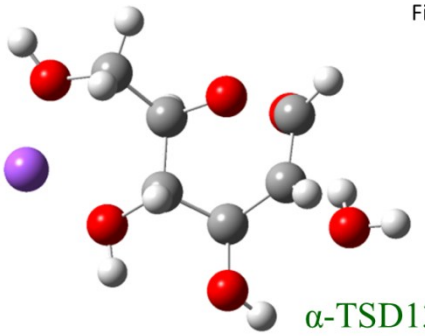

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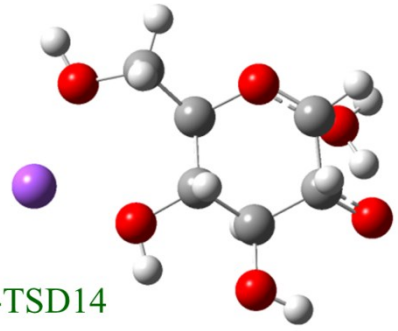

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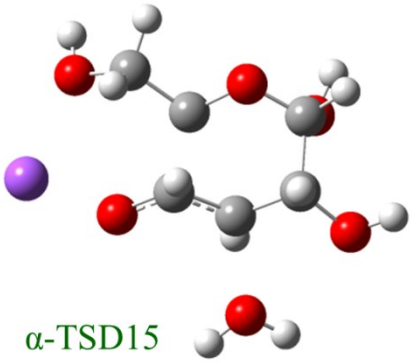

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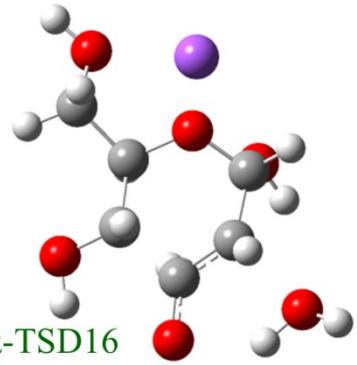

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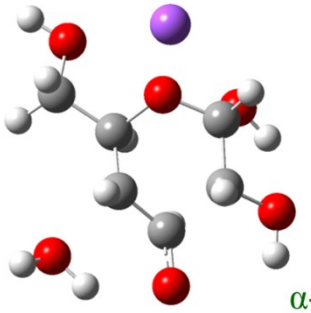

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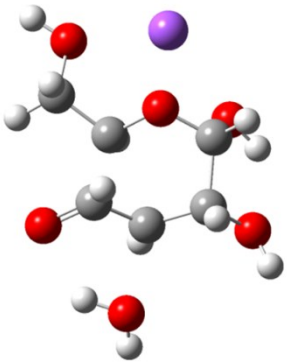

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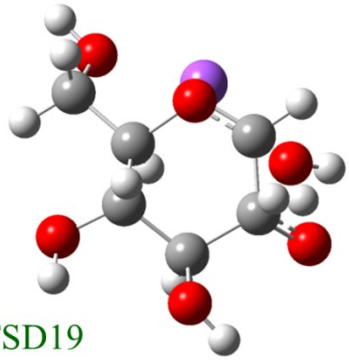

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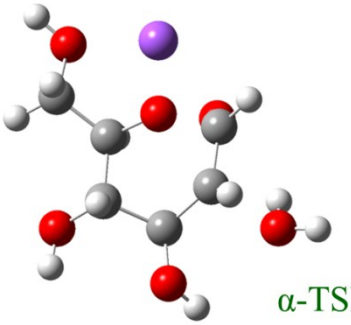

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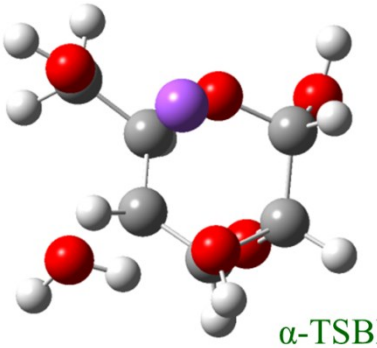

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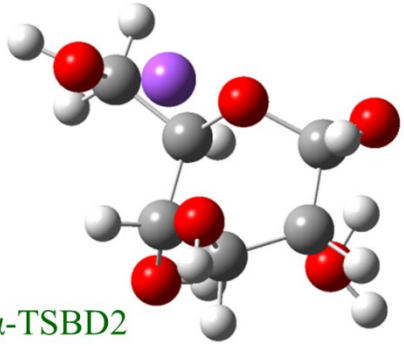

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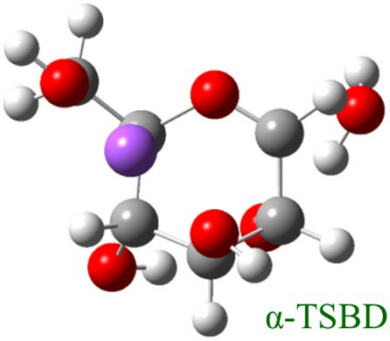

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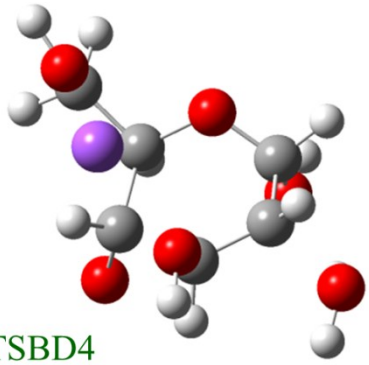

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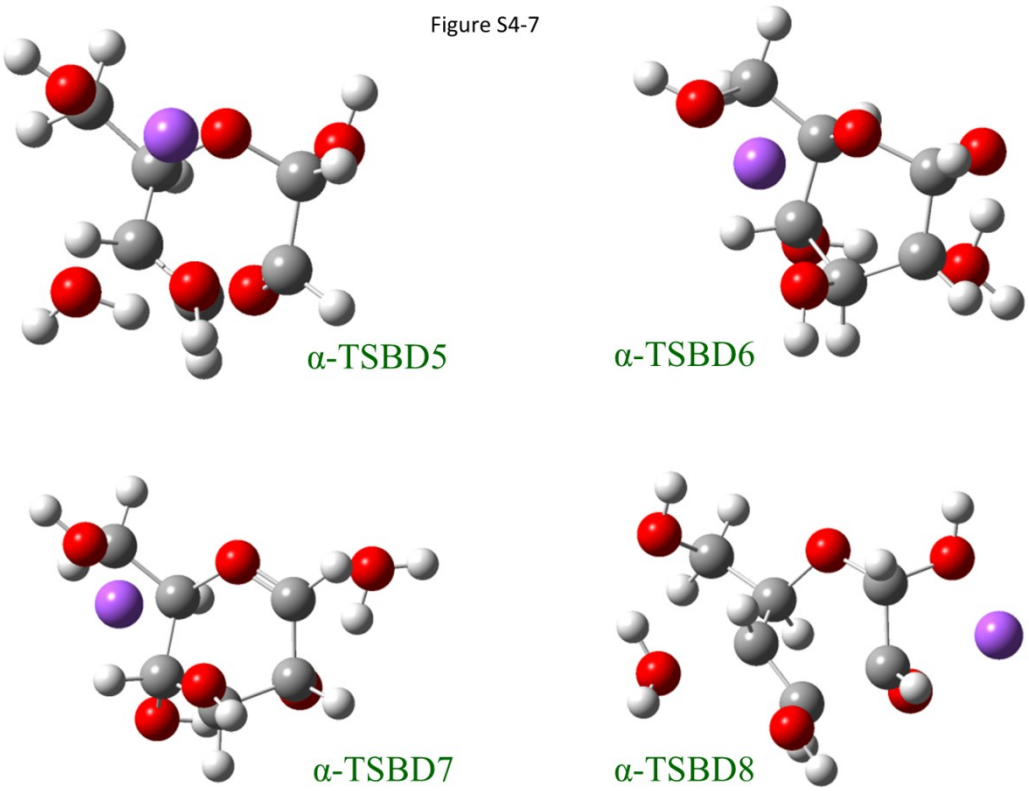

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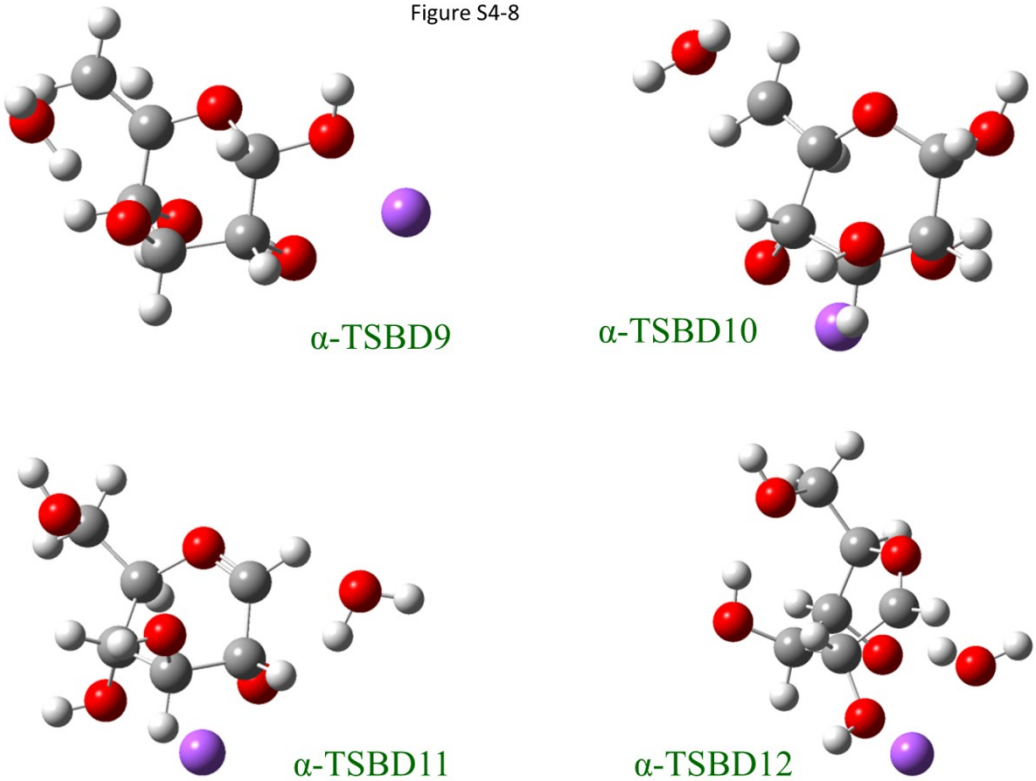
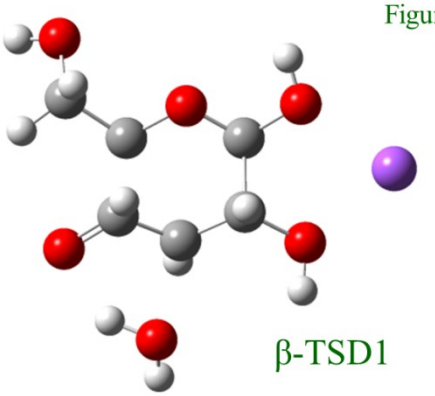


Figure S4. Transition state geometries of dehydration reactions of sodiated α-glucose.

Figure S5-1



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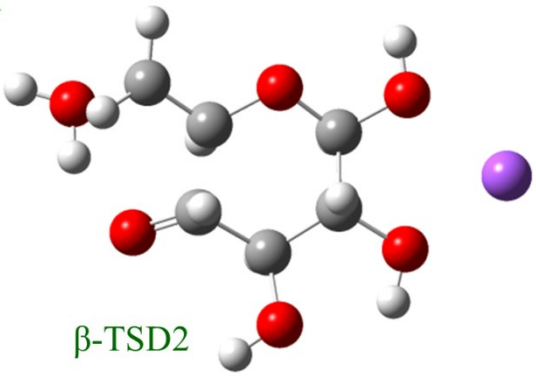

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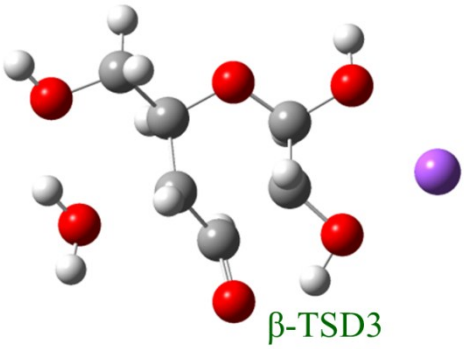

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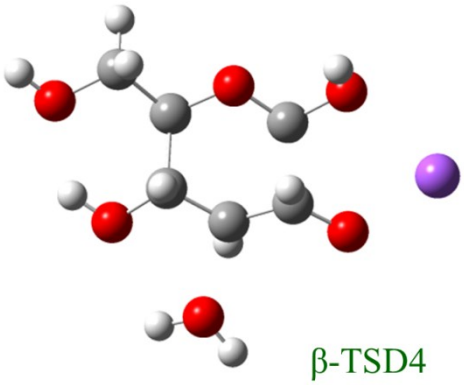

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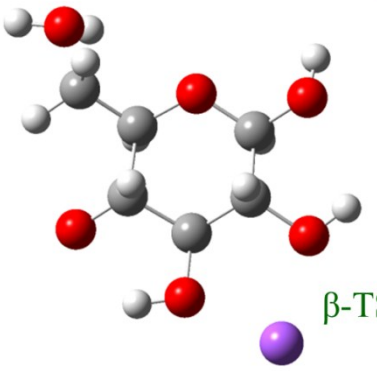

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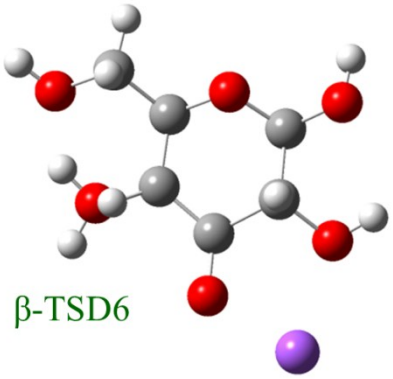

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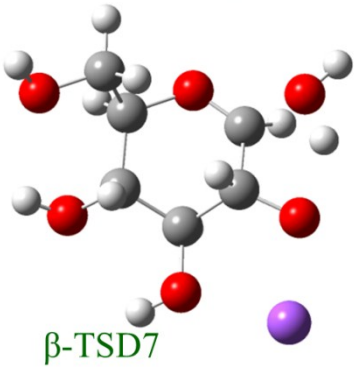

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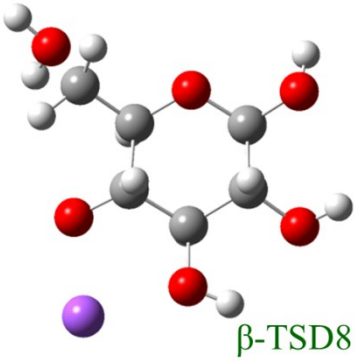

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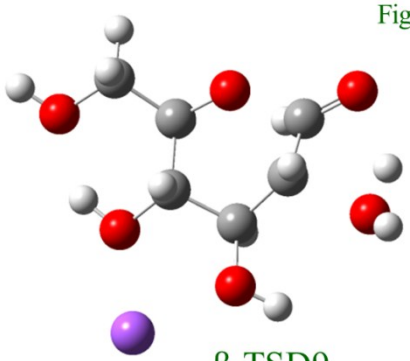

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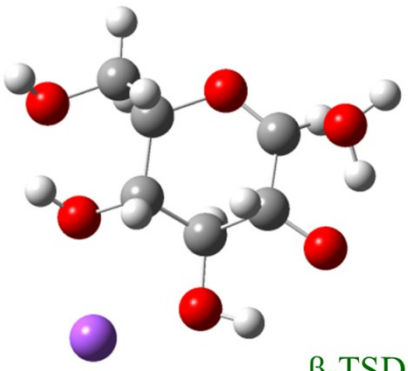

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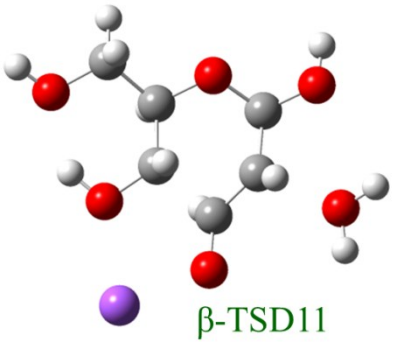

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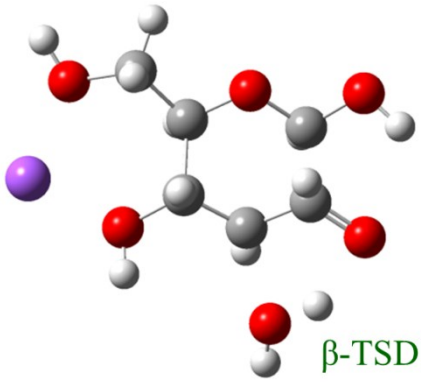

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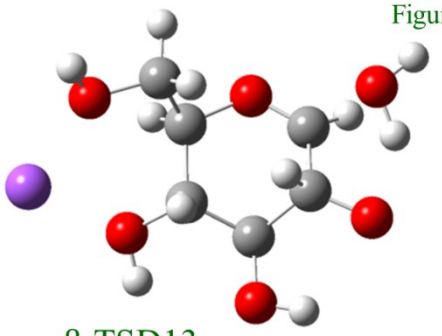

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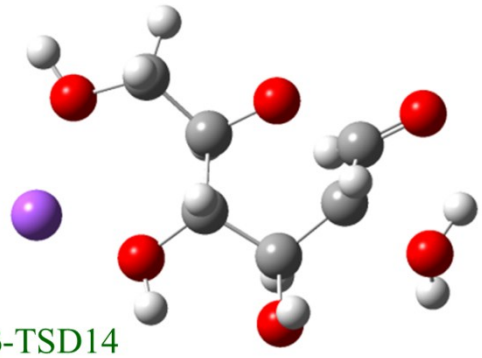

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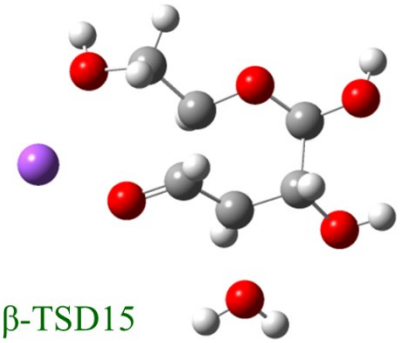

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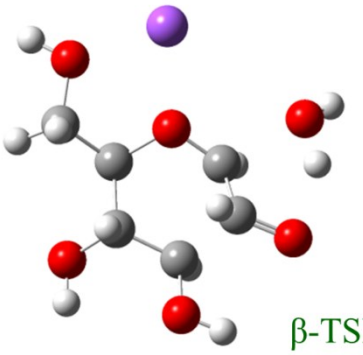

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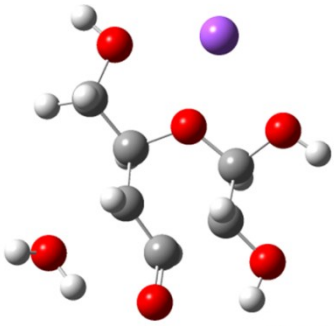

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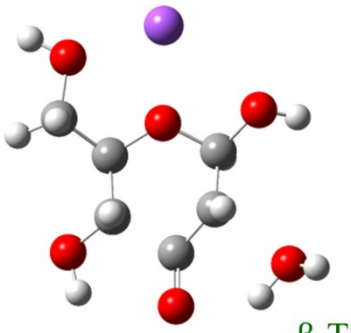

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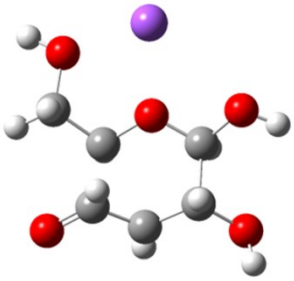

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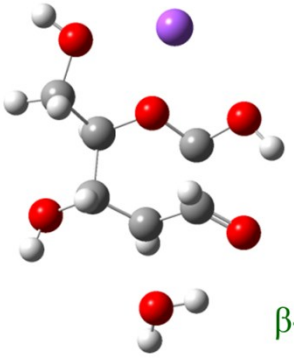

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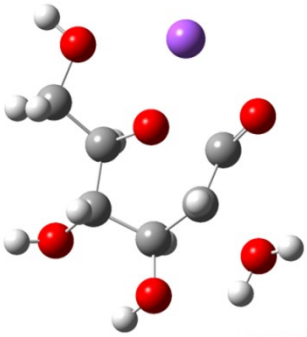

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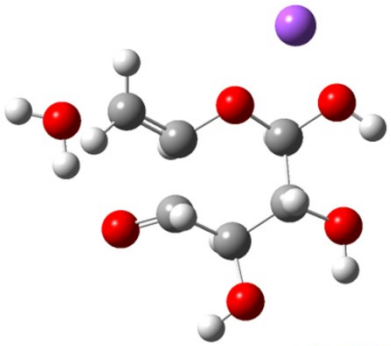

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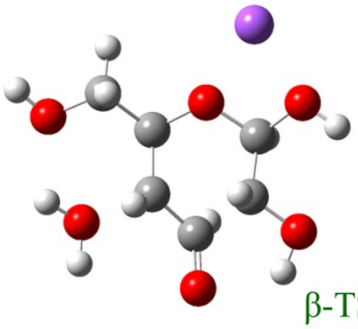

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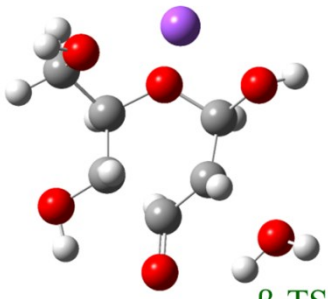

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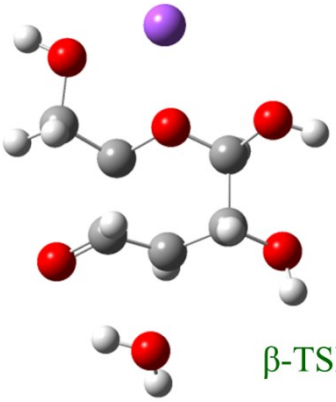
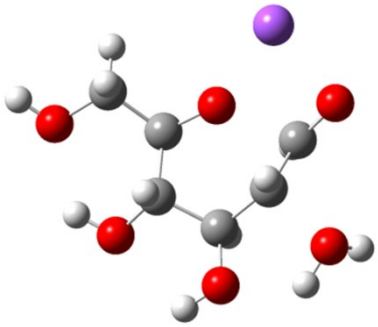
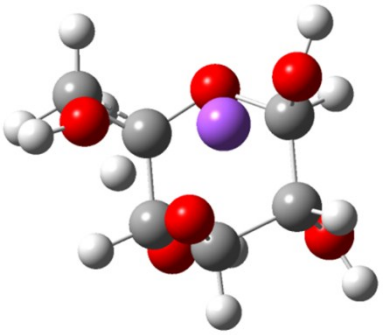


β-TSD25

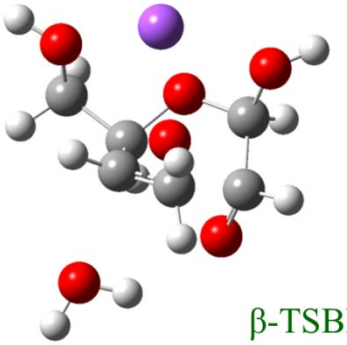


β-TSD26

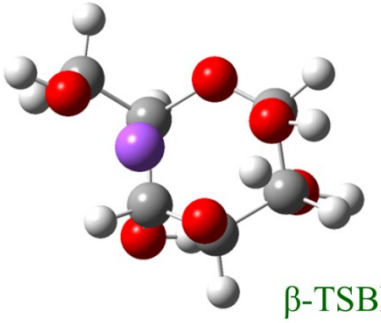
Figure S5-8



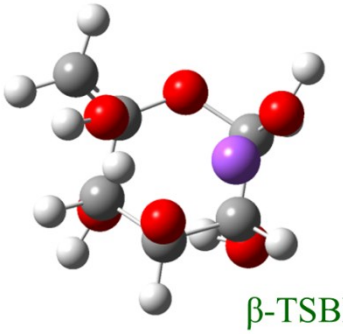
β-TSBD1



β-TSBD2



β-TSBD3



β-TSBD4

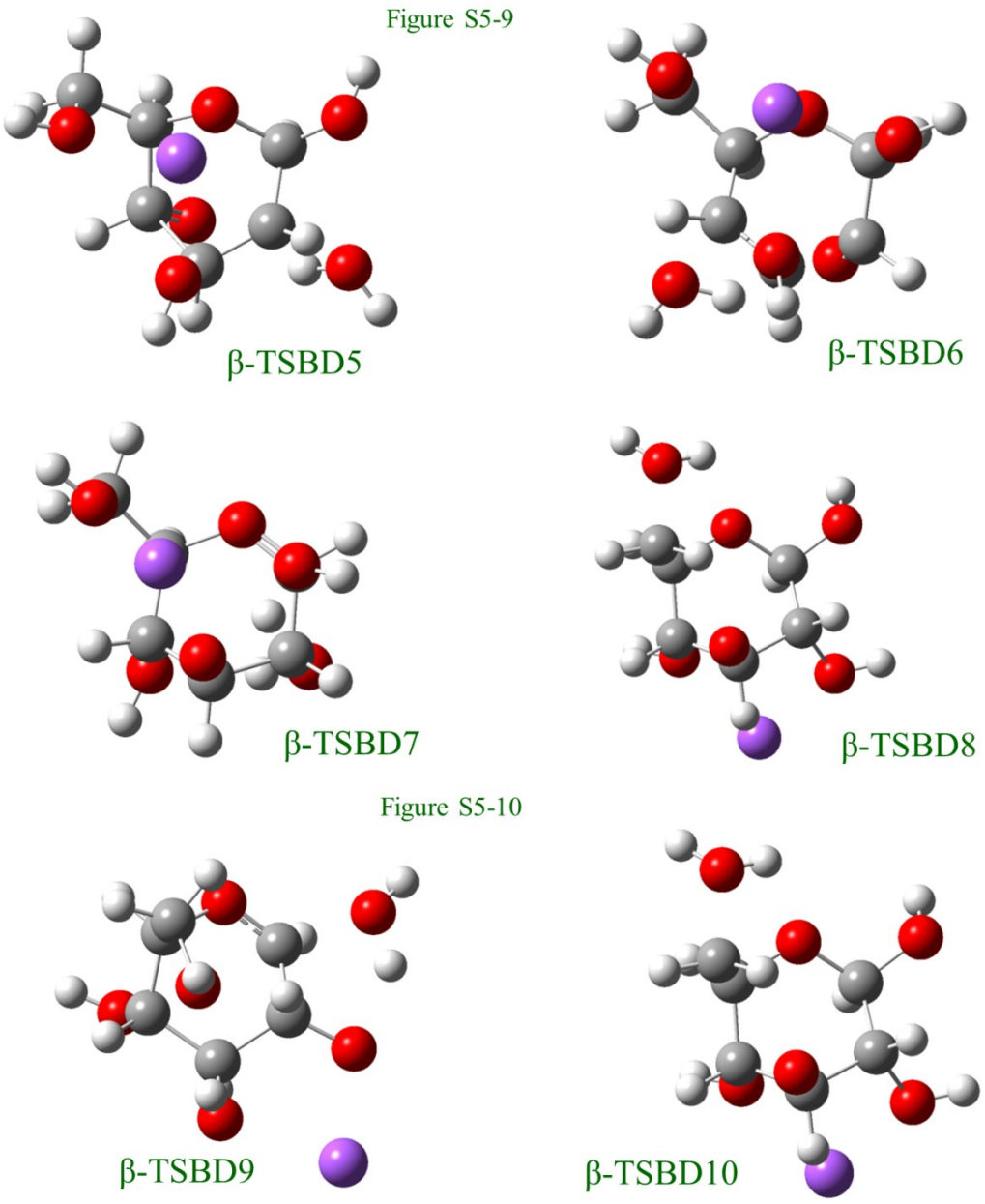
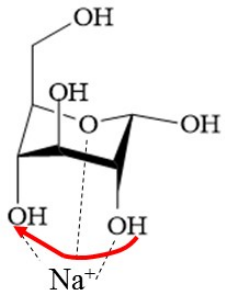
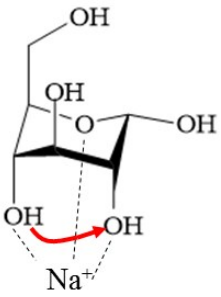


Figure S5. Transition state geometries of dehydration reactions of sodiated β-glucose.

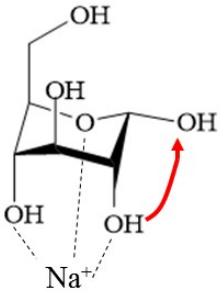
$^1C_4$ α-form



270.4 kJ/mol
(64.7 kcal/mol)

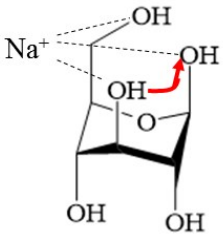


307.6 kJ/mol
(73.6 kcal/mol)

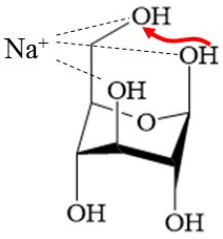


275.0 kJ/mol
(65.8 kcal/mol)

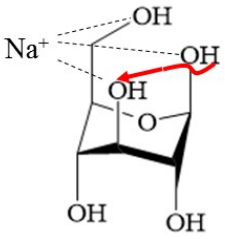
$^1C_4$ β-form



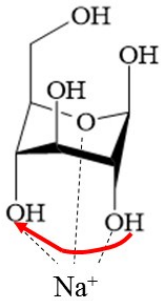
217.3 kJ/mol
(52.0 kcal/mol)



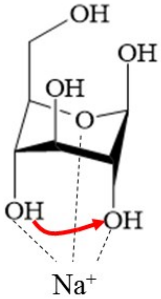
269.6 kJ/mol
(64.5 kcal/mol)



240.8 kJ/mol
(57.6 kcal/mol)



272.1 kJ/mol
(65.1 kcal/mol)



329.4 kJ/mol
(78.8 kcal/mol)

Figure S6. Energies of transition states for dehydration reaction of sodiated glucose with $^1C_4$ conformation.

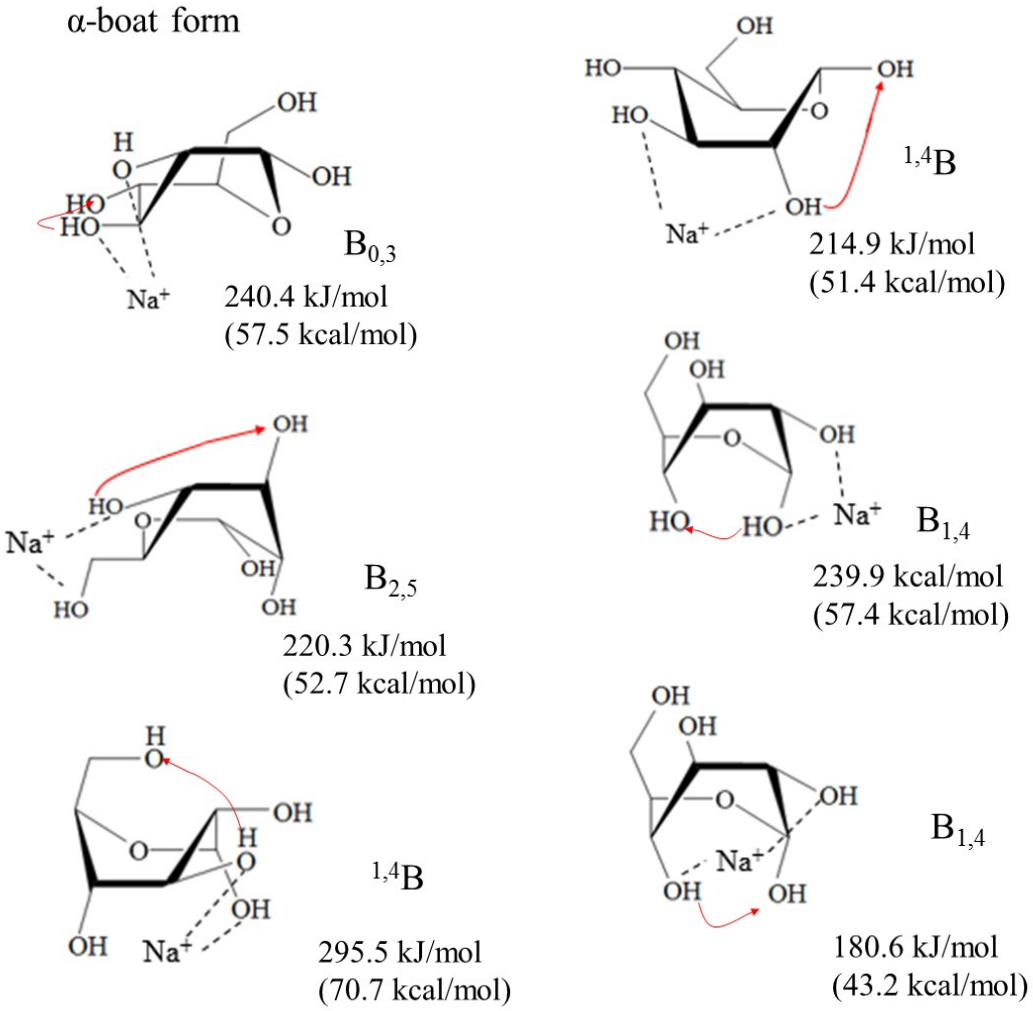


Figure S7-1. Energies of transition states of dehydration reaction for α-sodiated glucose of various boat conformations.

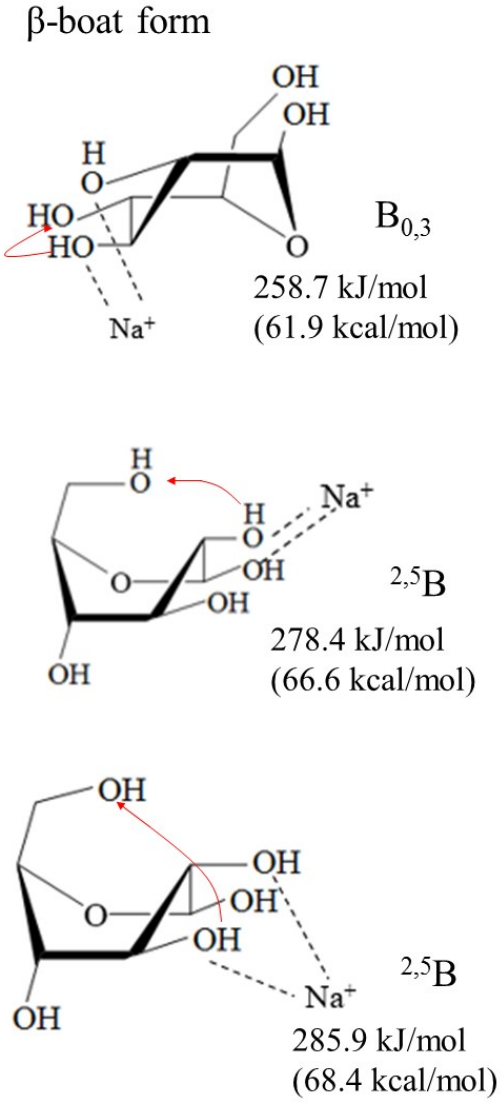


Figure S7-2. Energies of transition states of dehydration reaction for β-sodiated glucose of various boat conformations.

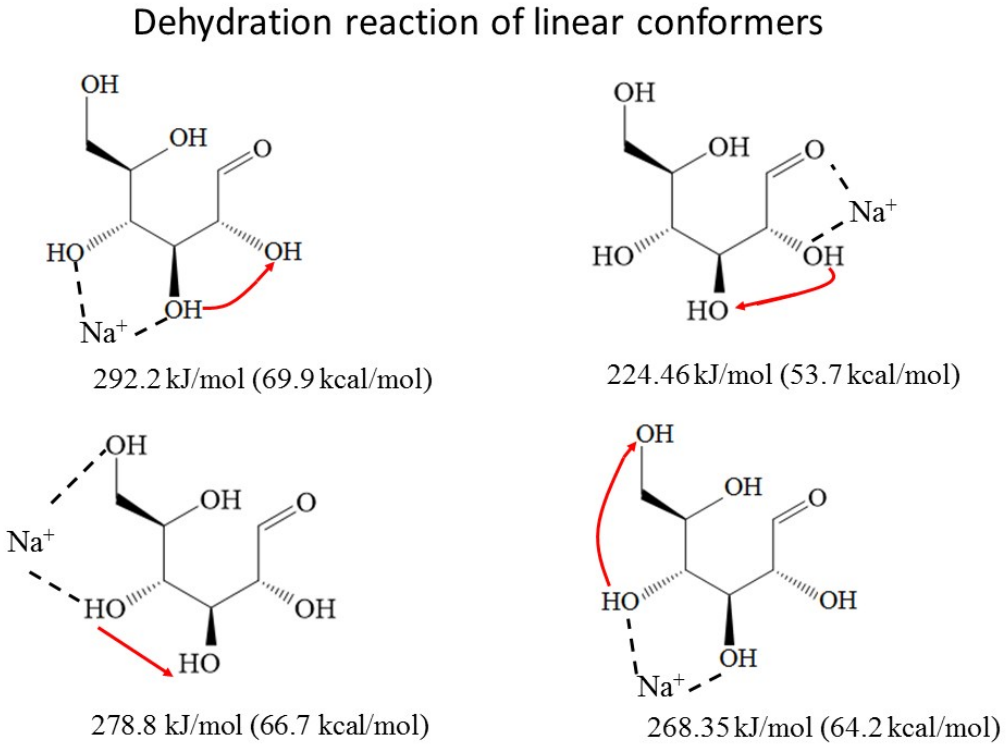


Figure S8. Transition state geometries and energies of linear conformer dehydration.

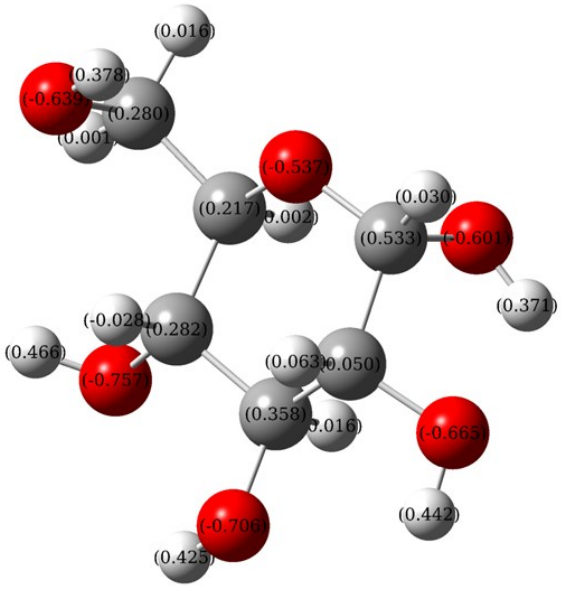


Figure S9-1. Charge distribution of glucose.

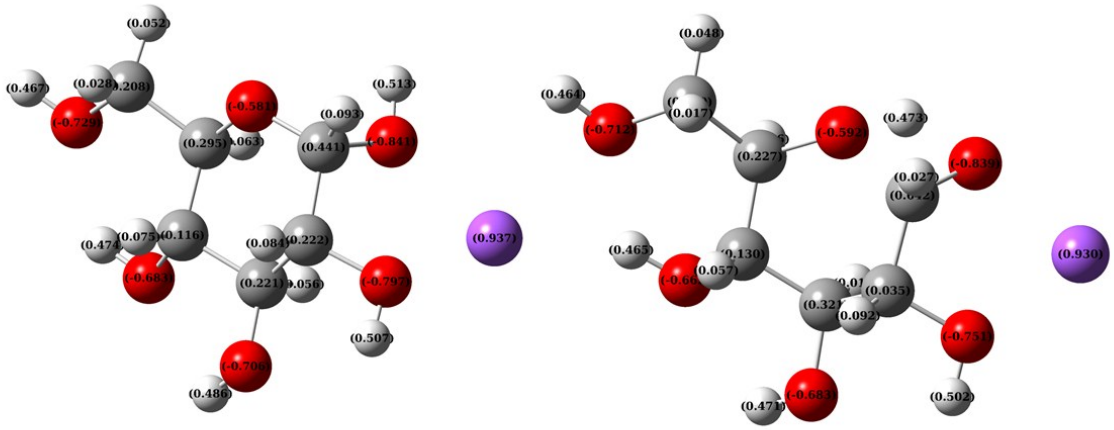
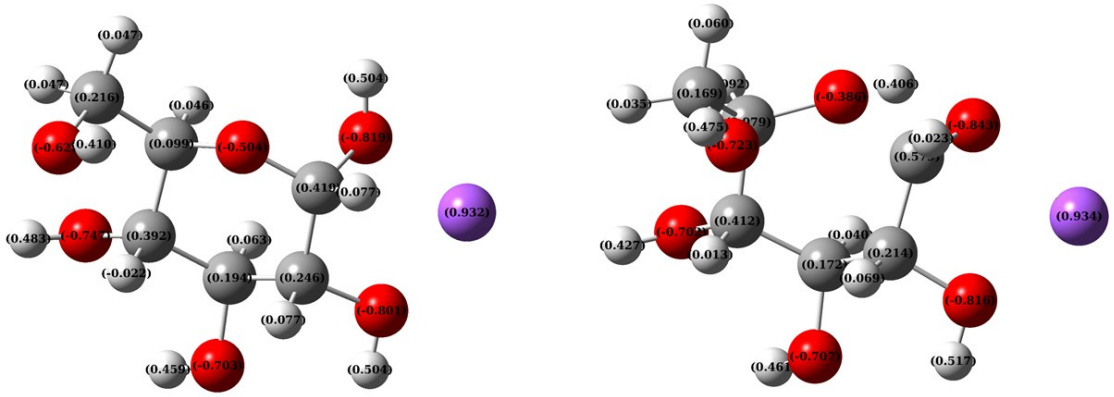
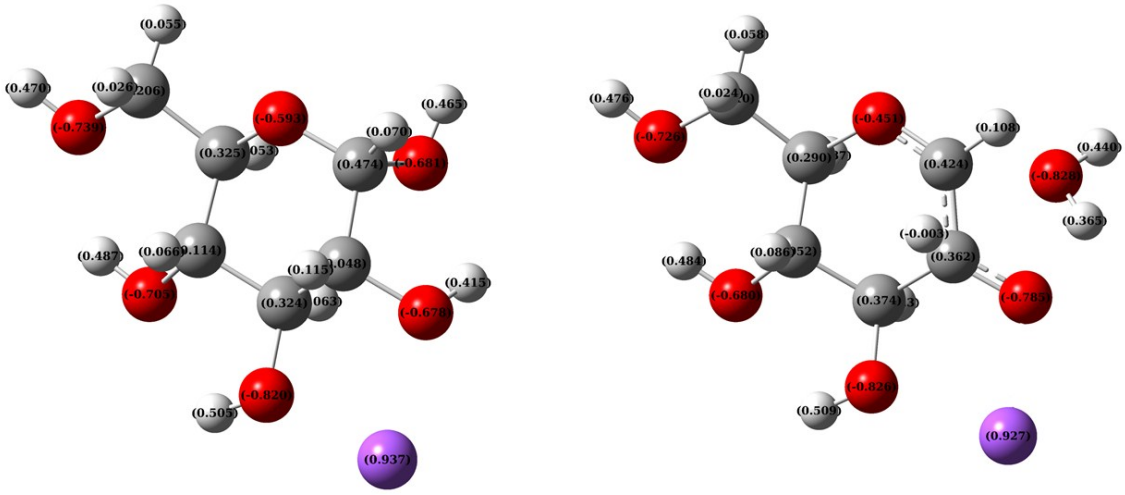


Figure S9-2. Charge distribution of sodiated glucose α-SG1 and the corresponding transition state for cross-ring dissociation.



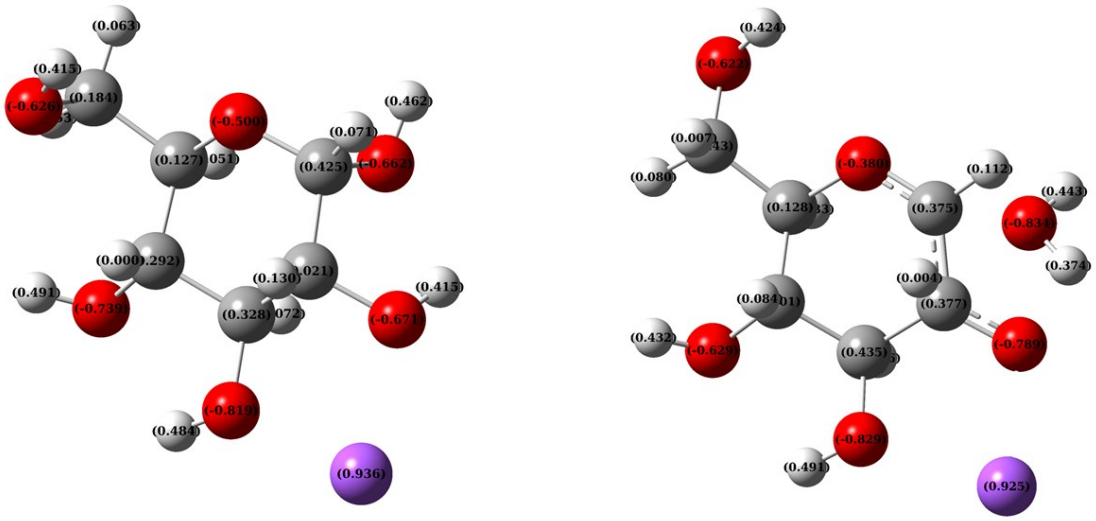
α-SG1'　　α-SG1'(-$C_2H_4O_2$)

Figure S9-3. Charge distribution of sodiated glucose α-SG1' and the corresponding transition state for cross-ring dissociation.



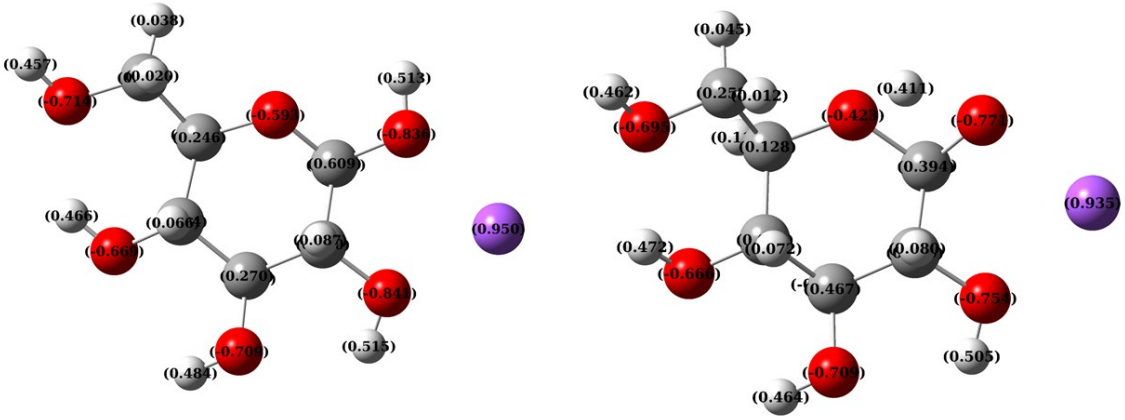
α-SG2　　α-SG2 (-H_2O)

Figure S9-4. Charge distribution of sodiated glucose α-SG2 and the corresponding transition state for dehydration.



α-SG2' α-SG2' (-H_2O)

Figure S9-5. Charge distribution of sodiated glucose α-SG2’ and the corresponding transition state for dehydration.



β-SG1 β-SG1 (-$C_2H_4O_2$)

Figure S9-6. Charge distribution of sodiated glucose β-SG1 and the corresponding transition state for cross-ring dissociation.

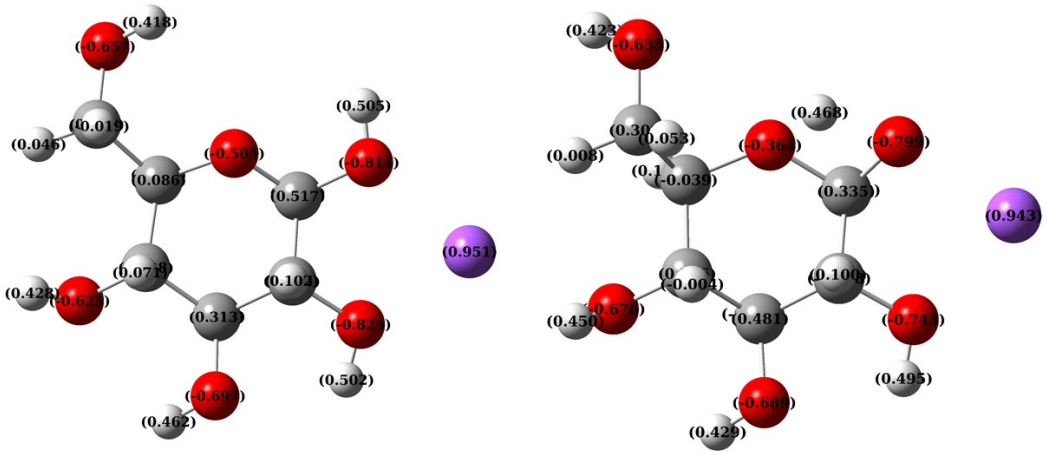


Figure S9-7. Charge distribution of sodiated glucose β-SG1' and the corresponding transition state for cross-ring dissociation.

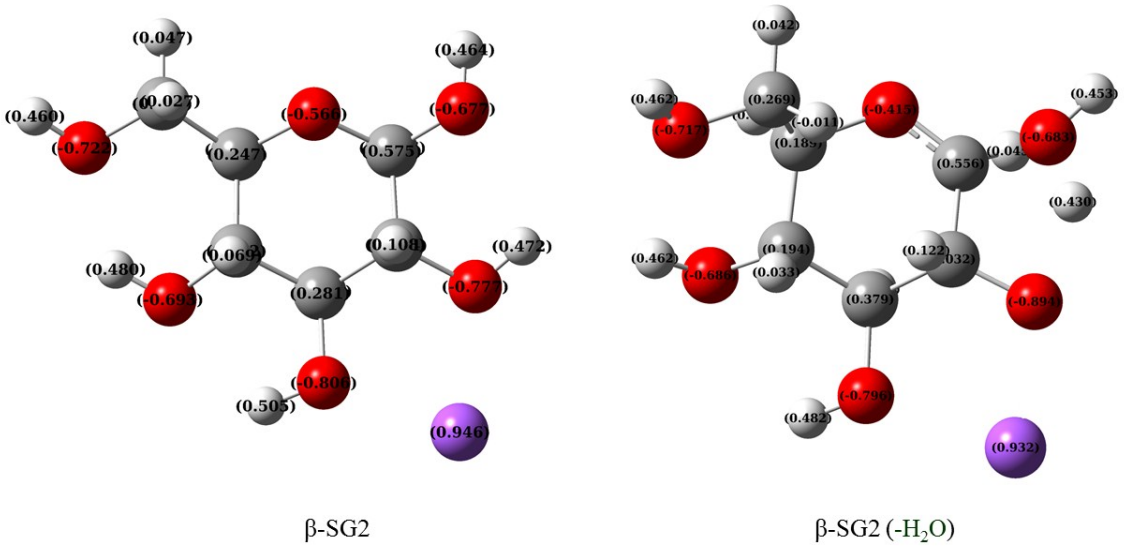


Figure S9-8. Charge distribution of sodiated glucose β-SG2 and the corresponding transition state for dehydration.

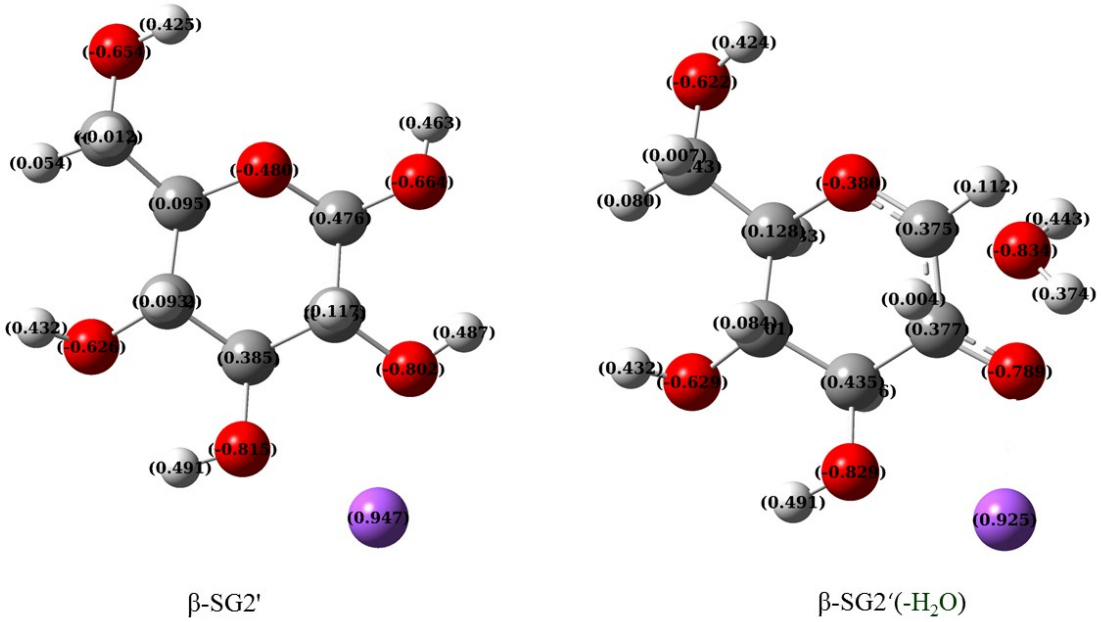


Figure S9-9. Charge distribution of sodiated glucose β-SG2’ and the corresponding transition state for dehydration.

Table SI. Energies (kJ/mol) of transition states for the first bond cleavage in cross ring dissociation. The number 40.7 in the upper-left corner represents the energy of transition state for the cleavage of #0 bond (C1-O0 bond) starting from geometry α-SG1. The number 79.3 and 86.1 in the upper-left corner represents the energies of transition states for the cleavage of #1 bond (C1-C2 bond), starting from geometry α-SG2 by transferring the H atom from O2and O1 to C1 and C2, respectively. The structures with the lowest barriers for each bond cleavage are shown in Figure S10.

	#0	#1		#2		#3		#4
α-SG1	170.4	X	X	377.6	434.9	409.7	416.1	417.3
α-SG2	185.0	328.8	357.4	X	X	358.8	410.6	387.6
α-SG3	187.1	336.2	379.7	395.3	358.2	X	X	356.5
α-SG4	208.5	357.2	402.9	398.3	398.8	416.1	353.6	X
α-SG5	215.6	339.9	402.1	364.7	382.0	381.8	379.4	392.8
β-SG 1	190.0	X	X	382.7	430.5	409.9	409.4	414.5
β-SG 2	208.0	341.2	359.6	X	X	366.8	416.6	390.4
β-SG 3	191.7	348.6	393.3	413.1	365.6	X	X	359.4
β-SG 4	202.2	370.1	418.4	425.3	408.5	432.6	364.6	X
β-SG 5	213.9	346.7	408.4	388.5	385.0	393.8	385.2	403.7
β-SG 6	X	366.6	476.7	442.6	453.1	439.9	424.3	441.9
α-BG1	198.8	367.0	406.8	418.9	365.4	X	392.6	393.0
α-BG2	174.2	X	X	413.1	431.4	413.1	423.1	395.2
α-BG3	215.1	355.1	387.7	X	X	X	X	370.7
α-BG4	202.5	359.2	406.5	395.5	366.6	371.9	404.0	376.2
β-BG 1	190.5	336.7	396.0	404.4	358.7	364.5	397.7	373.6
β-BG 2	201.8	X	X	368.9	428.1	420.8	420.2	418.0
β-BG 3	267.5	395.7	394.1	X	X	X	X	370.2
β-BG 4	189.6	344.6	396.0	402.0	365.7	364.5	397.7	373.6

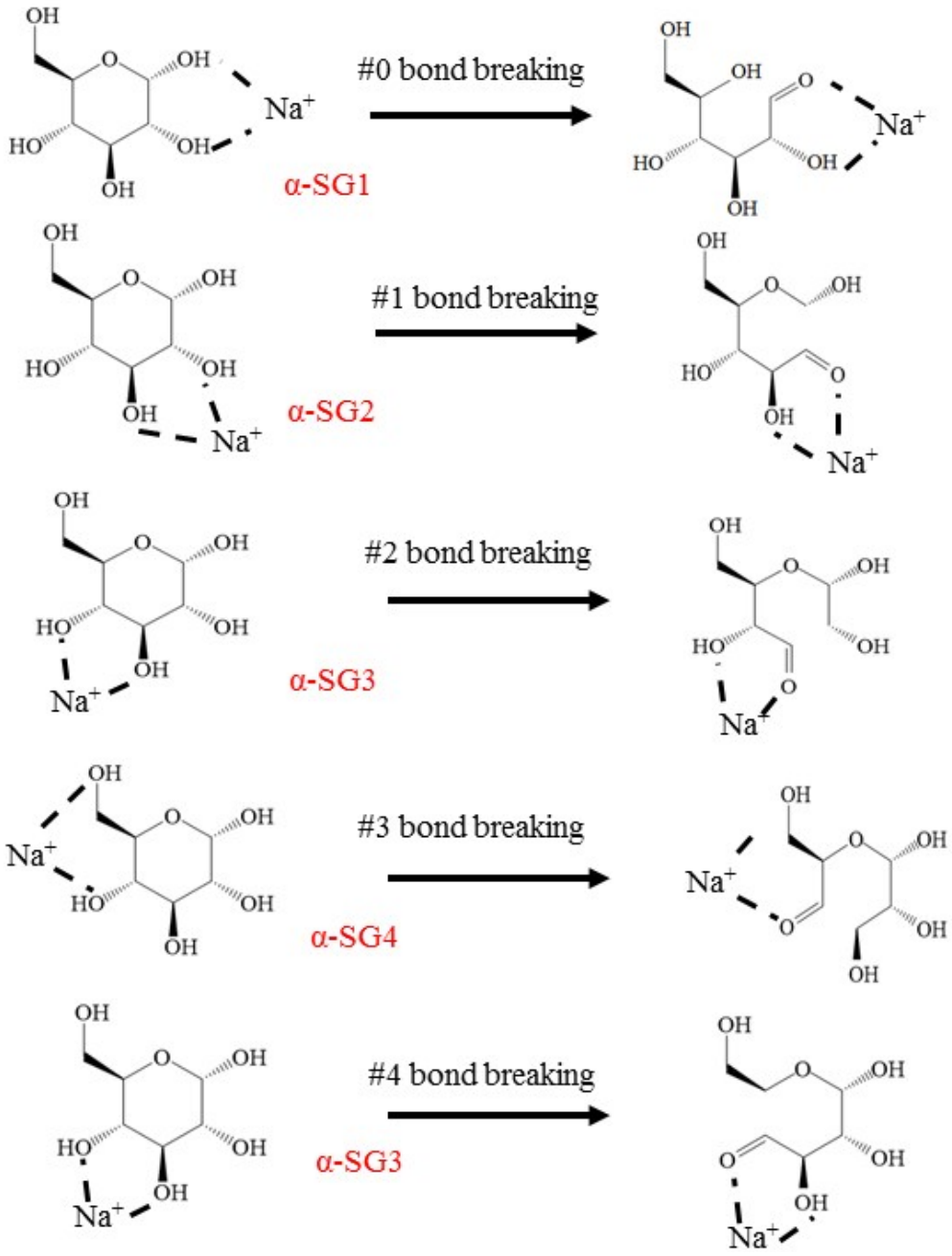


Figure S10. The scheme of structures with the lowest barriers in Table S1 for each bond cleavage.

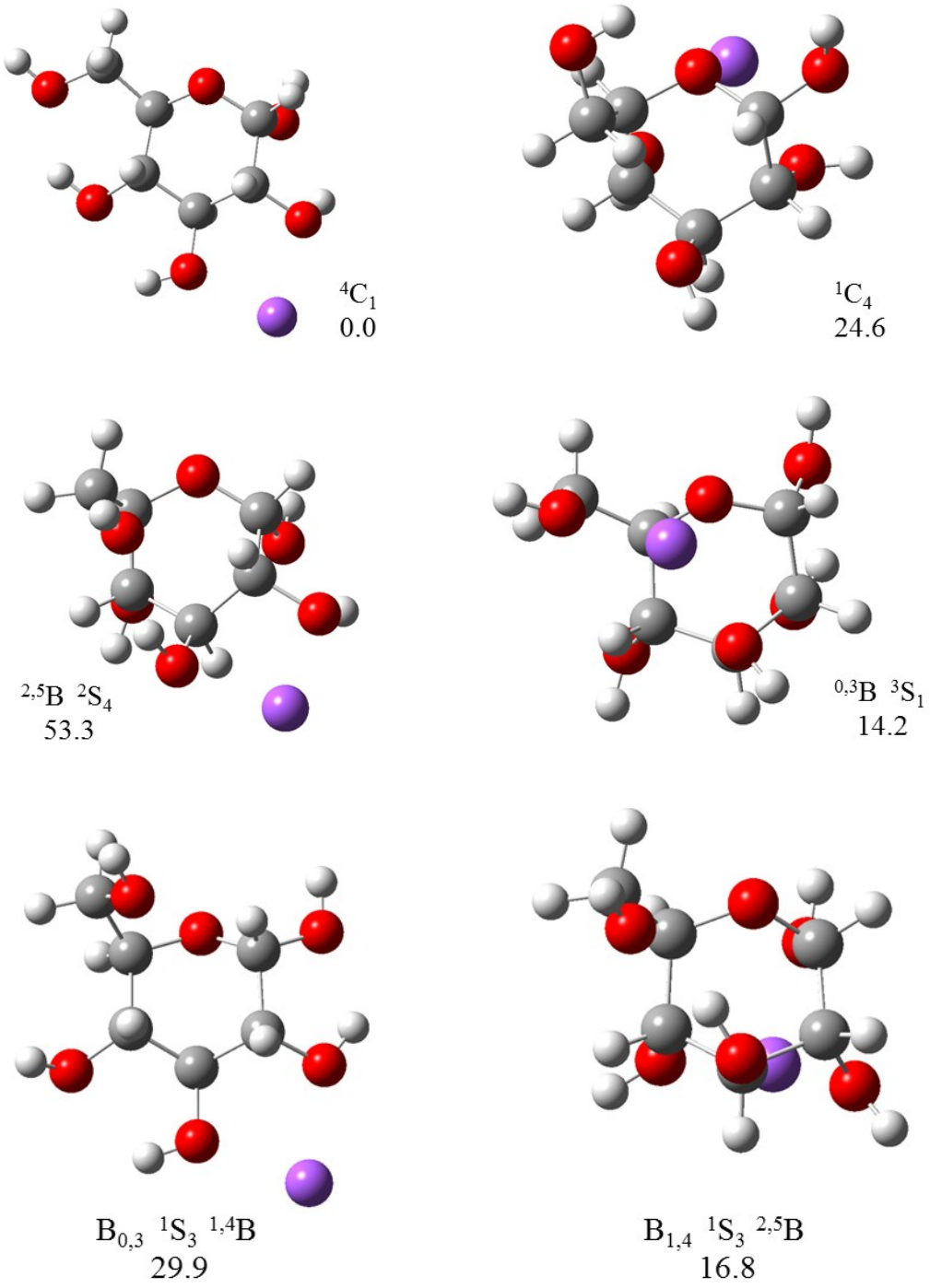


Figure S11-1. Geometries and energies (B3LYP/6-311+G(d,p), kJ/mol) of sodiated α-glucoses used in the search for dissociation of low barriers. The geometries of sodiated glucose starting from the types of $^{4}C_{1}$ and $^{0,3}B$ are shown in Figure 3 and 4. The other types are shown here.

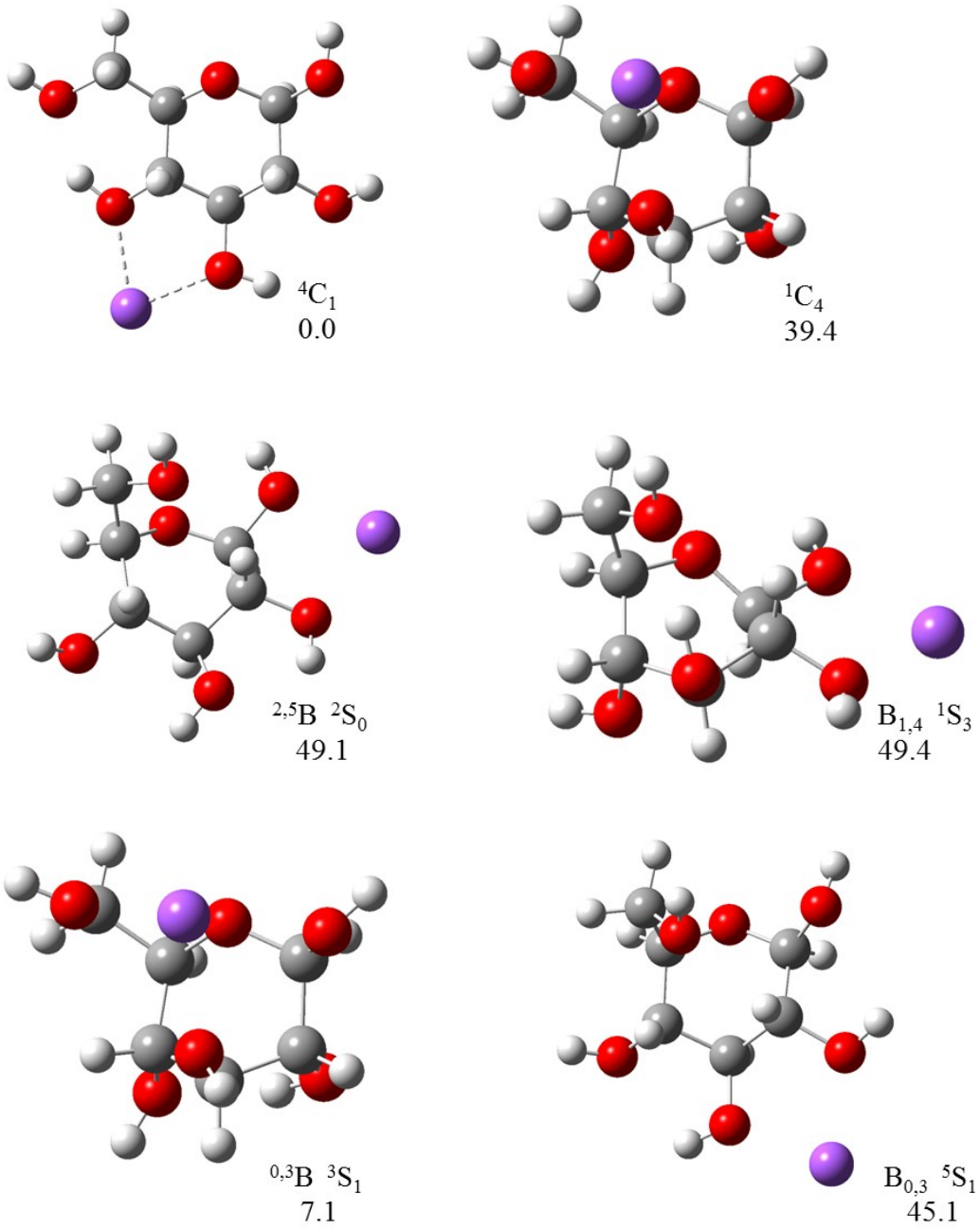


Figure S11-2. Geometries and energies (B3LYP/6-311+G(d,p), kJ/mol) of sodiated β-glucoses used in the search for dissociation of low barriers. The geometries of β-sodiated glucose starting from the types of $^{4}C_{1}$ and $^{0,3}B$ are shown in Figure S2 and S3. The other types are shown here.

Table S2. The XYZ coordinates of each atom for the sodiated glucose shown in Figure 7.

α-SG1

C	0.87978800	-1.15299900	-0.69401700
C	-1.37056100	-0.66880200	0.10615500
C	1.16215200	0.34188500	-0.86203100
C	0.29878700	1.19032000	0.05579500
C	-1.17498200	0.84075100	-0.12042800
O	-0.47578200	-1.43688800	-0.74040800
O	2.56229200	0.59598100	-0.61690600
O	0.59453800	2.53748000	-0.26943000
O	-1.86380400	1.62749500	0.83087700
H	-1.17371400	-0.89713700	1.15933700
H	0.93787600	0.59839400	-1.90151800
H	2.71428500	1.52731300	-0.83049300
H	0.56140100	0.99039000	1.10508600
H	-0.01983200	3.11129000	0.20662100
H	-1.48717800	1.09565900	-1.14419300
H	-2.79135700	1.34622000	0.84559500
C	-2.76408100	-1.16159300	-0.27840100
H	-2.85162400	-2.22710600	-0.04375800
H	-2.90567300	-1.02609400	-1.35680900
O	-3.70195000	-0.38633600	0.46841200
H	-4.59919200	-0.67340800	0.27110100
Na	3.47013100	-0.61613400	1.03564800
H	1.32662900	-1.72836100	-1.50769100
O	1.48104600	-1.58715400	0.55632300
H	1.15960700	-2.48167700	0.73121800

α-SG1 (-$C_2H_4O_2$)

C	-1.06539400	-1.05603900	0.66353700
C	1.45206400	-0.71129400	-0.33560400
C	-1.11665300	0.47333700	0.79817600
C	-0.18148500	1.19717800	-0.15943900
C	1.26203800	0.75818400	0.07709700
O	0.29728100	-1.54431900	0.05545400
O	-2.48355400	0.85680200	0.55512900

O	-0.36904700	2.57360400	0.10212100
O	2.06360000	1.60403200	-0.72120700
H	1.50276400	-0.75439900	-1.42539400
H	-0.85065000	0.75784500	1.82136700
H	-2.52445300	1.81725300	0.66798500
H	-0.45525000	0.96691100	-1.19997000
H	0.33162500	3.06946400	-0.34309700
H	1.50981600	0.88527900	1.14103400
H	2.99188800	1.36512000	-0.58318800
C	2.68665500	-1.35694200	0.28854000
H	2.83178200	-2.35992900	-0.12473900
H	2.54295200	-1.43972900	1.37303000
O	3.77755200	-0.49502700	-0.02504700
H	4.60797100	-0.88346300	0.26878600
Na	-3.72708800	-0.63121800	-0.68705900
H	-1.12192900	-1.57566500	1.62400600
O	-1.79324400	-1.60019600	-0.33782400
H	-0.53259400	-1.89100600	-0.68500500

α-SG1′

C	0.57592000	-1.16862400	-0.56213700
C	-1.46367400	-0.26968800	0.43300500
C	1.07534400	0.24658100	-0.86735300
C	0.43988100	1.29399600	0.03486300
C	-1.08055200	1.15781500	0.01464400
O	-0.80688300	-1.21926900	-0.45184300
O	2.51277700	0.27987200	-0.75076500
O	0.90132500	2.54216400	-0.44858800
O	-1.56271000	2.11939500	0.94347900
H	-1.10656600	-0.43644100	1.45326000
H	0.80402700	0.46674500	-1.90428600
H	2.79588300	1.15433500	-1.05288900
H	0.77209300	1.14284200	1.07252200
H	0.47821100	3.24677900	0.05836500
H	-1.45574100	1.36303100	-0.99588700
H	-2.46105900	2.38568900	0.72102000
C	-2.99441900	-0.55179000	0.35843500

H	-3.51107300	0.38021300	0.09286000
H	-3.35242500	-0.84648400	1.34779000
O	-3.36845700	-1.55564400	-0.56155700
H	-2.60100200	-1.81873300	-1.08056100
Na	3.40794100	-1.02554200	0.84029500
H	0.82910600	-1.85347400	-1.37456300
O	1.22692800	-1.63005700	0.64819100
H	0.78234900	-2.44497600	0.91904600

α-SG1′ (-$C_2H_4O_2$)

C	-0.79152700	-1.17789300	0.20279700
C	1.65680600	-0.50479500	-0.71758400
C	-0.79068200	0.22792200	0.82285800
C	-0.10009200	1.23988500	-0.08520900
C	1.39311900	0.93176300	-0.19694400
O	0.43612500	-1.33955700	-0.71481100
O	-2.17307600	0.58499300	1.01042700
O	-0.32644100	2.50678500	0.50697800
O	1.94298400	1.89039600	-1.09810300
H	1.94105700	-0.44829100	-1.76841600
H	-0.29035100	0.20867000	1.79556800
H	-2.17846600	1.48171600	1.37424700
H	-0.54780300	1.20581300	-1.08841600
H	0.09533700	3.18455400	-0.03566200
H	1.83389600	1.04459800	0.79695600
H	2.80356300	2.18938300	-0.78786200
C	2.70875100	-1.25353500	0.07831000
H	3.66315900	-0.71746300	-0.01146100
H	2.83343200	-2.25891400	-0.33605000
O	2.25466100	-1.29533400	1.42675800
H	2.86414600	-1.81082700	1.96465700
Na	-3.63473500	-0.48976100	-0.41702700
H	-0.72752100	-1.98253700	0.93876800
O	-1.67258200	-1.36227000	-0.81138200
H	-0.45997200	-1.36951700	-1.43934100

α-SG2

C	-0.29485600	1.82458900	-0.28496900
C	1.62533600	0.39271700	0.11743500
C	-1.20347900	0.60270100	-0.50466600
C	-0.64190000	-0.60277100	0.23037700
C	0.79637000	-0.86905400	-0.18512600
O	1.04486200	1.52332800	-0.56344200
O	-2.55364800	0.87113500	-0.07350100
O	-1.48725100	-1.74152000	-0.05411600
O	1.18730700	-2.01458000	0.54790100
H	1.63593300	0.56460400	1.19903200
H	-1.25482700	0.39418900	-1.57589700
H	-2.49387100	1.50932900	0.65502300
H	-0.65970400	-0.42181500	1.31051200
H	-0.97319700	-2.53231200	0.16862500
H	0.83814300	-1.06633400	-1.26732100
H	2.15083100	-2.10840600	0.47652800
C	3.05521700	0.31113300	-0.41080100
H	3.60780400	1.20246100	-0.09975700
H	3.03294500	0.27435400	-1.50591700
O	3.63566300	-0.87733200	0.13329600
H	4.56234000	-0.93967600	-0.11868600
Na	-3.64957400	-1.12925700	-0.14504100
O	-0.52970100	2.22241700	1.05333500
H	-0.14723200	3.09401400	1.21147800
H	-0.55183700	2.62793600	-0.97945900

α-SG2 (-H_2O)

C	-0.33552500	1.51501100	-0.82205900
C	1.64531900	0.48792600	0.08241600
C	-1.21253100	0.42099600	-0.47701800
C	-0.52677400	-0.71356900	0.28011500
C	0.94289900	-0.86828100	-0.08905600
O	0.96267600	1.52112400	-0.71970100
O	-2.49783800	0.54787800	-0.37742800
O	-1.26583900	-1.92052600	0.03736700
O	1.44848700	-1.85670500	0.78297500
H	1.59593700	0.80983900	1.12533200
H	-0.84604900	0.32801700	-1.68284800

H	-2.30514000	2.21342000	1.02532500
H	-0.58741600	-0.46406200	1.34601400
H	-0.74730700	-2.65162100	0.40234900
H	1.03018000	-1.19135700	-1.13805300
H	2.41556600	-1.87977000	0.70624300
C	3.08398900	0.51592800	-0.43041500
H	3.52629300	1.49264100	-0.21307400
H	3.08331200	0.36279900	-1.51632200
O	3.77423200	-0.53512300	0.23987300
H	4.71643100	-0.49474000	0.04626100
Na	-3.51472400	-1.37595900	-0.21416500
O	-1.46799900	2.57905300	1.34684100
H	-1.68033900	3.38794600	1.82286900
H	-0.75351500	2.38876300	-1.31159900

α-SG2′

C	-0.11622000	-1.65804300	-0.31225700
C	-1.62007200	0.19515900	0.13830500
C	1.06732900	-0.69566100	-0.50710900
C	0.81733400	0.61108700	0.23192000
C	-0.51725300	1.22016800	-0.17769400
O	-1.33167000	-1.02091100	-0.59246700
O	2.30430500	-1.28862000	-0.06463900
O	1.92030200	1.49997900	-0.05522300
O	-0.61084200	2.42760400	0.57180500
H	-1.63238100	-0.01624200	1.21229300
H	1.18099200	-0.49624800	-1.57542200
H	2.08009900	-1.90624400	0.64966100
H	0.79194400	0.42839000	1.31194000
H	1.63272900	2.39073700	0.19435000
H	-0.51346800	1.43319800	-1.25529100
H	-1.28798900	3.00671500	0.20615200
C	-3.01501200	0.62484000	-0.30104400
H	-3.01973200	0.79570100	-1.38644200
H	-3.27482200	1.56145700	0.19791500
O	-4.00113500	-0.30859800	0.08318600
H	-3.88235100	-1.11290200	-0.43357000

Na	3.87441900	0.36084000	-0.12727000
O	0.00262800	-2.12085800	1.01920000
H	-0.59966200	-2.85940500	1.17117200
H	-0.05930100	-2.48845700	-1.02039800

α-SG2′ (-H_2O)

C	0.04612700	1.34833600	-0.87246100
C	1.65862300	-0.13859500	0.12091100
C	-1.09611100	0.55215600	-0.48715700
C	-0.74700200	-0.71910700	0.28970900
C	0.63126900	-1.26564200	-0.06576200
O	1.29320900	0.99319400	-0.76810200
O	-2.29360200	1.02860800	-0.38382000
O	-1.78930800	-1.67659400	0.05055900
O	0.85395300	-2.34827700	0.82650400
H	1.62413400	0.25465500	1.13957600
H	-0.78259700	0.32916200	-1.69416300
H	-1.56071300	2.62922500	1.08807000
H	-0.74237000	-0.44870600	1.35224200
H	-1.51377800	-2.50811400	0.46093900
H	0.63821700	-1.61371300	-1.10733000
H	1.51405300	-2.95647600	0.47643600
C	3.09201600	-0.49703900	-0.24470300
H	3.14423700	-0.78188000	-1.30417800
H	3.39113500	-1.35802800	0.35749300
O	3.99494400	0.53699800	0.07128800
H	3.91691500	1.24634600	-0.57560000
Na	-3.81434900	-0.51887300	-0.20262200
O	-0.62892200	2.65228800	1.34556200
H	-0.50039800	3.46051600	1.85237100
H	-0.12270900	2.28422300	-1.39616200

β-SG1

C	0.94445700	-0.89691000	0.37439600
C	-1.42770100	-0.72613200	0.30057600
C	1.12982500	0.47767500	-0.25123700
C	-0.01571500	1.36368000	0.20209000

C	-1.35400900	0.73725400	-0.19818000
O	2.02311100	-1.73140700	-0.03827600
O	-0.24557400	-1.46056300	-0.09650000
O	2.40754400	1.01857600	0.14007800
O	0.21487800	2.63309200	-0.38369800
O	-2.34112200	1.55710300	0.39197600
H	0.93471800	-0.83414900	1.47312000
H	1.73703700	-2.65215800	0.03451800
H	-1.50627700	-0.72008000	1.39549300
H	1.10649600	0.36761500	-1.34104400
H	2.34218200	1.98282900	0.06694800
H	0.00001100	1.45039100	1.29853900
H	-0.50748000	3.22530300	-0.13790200
H	-1.43563200	0.74606300	-1.29494800
H	-3.20632200	1.14903600	0.23750500
C	-2.59646100	-1.50420900	-0.29923000
H	-2.64398400	-2.49843100	0.15596500
H	-2.43338200	-1.61641100	-1.37750000
O	-3.77944200	-0.75264700	-0.03117900
H	-4.55166700	-1.21924800	-0.36597100
Na	3.98606900	-0.56383000	-0.07040300

β-SG1 (-$C_2H_4O_2$)

C	1.17899600	-0.76062600	0.63216800
C	-1.46626200	-0.70205800	0.43882600
C	1.13931000	0.54700800	-0.14189200
C	-0.02153400	1.41592200	0.30161700
C	-1.32107300	0.72525700	-0.14322200
O	1.86140500	-1.75015500	0.01237200
O	-0.17298800	-1.42430700	0.49073400
O	2.43721900	1.13038100	0.03511100
O	0.15495800	2.66916400	-0.32883800
O	-2.37430900	1.54148200	0.32060200
H	1.37461500	-0.62281100	1.70257900
H	0.50194600	-2.09720300	-0.15525500
H	-1.78909500	-0.62112200	1.47830600
H	1.00568800	0.30743900	-1.20498800
H	2.36505700	2.08219800	-0.12981500

H	-0.03232200	1.53525000	1.39448400
H	-0.59744200	3.23761200	-0.11914800
H	-1.31952100	0.67822700	-1.24121200
H	-3.21194600	1.17290500	0.00493500
C	-2.42923700	-1.58447800	-0.35159600
H	-2.57737100	-2.53430300	0.17200400
H	-2.00940200	-1.78635800	-1.34604600
O	-3.63879000	-0.84242900	-0.44893000
H	-4.33434700	-1.38306900	-0.83736900
Na	3.81845200	-0.76436300	-0.43475300

β-SG1′

C	0.71314000	-0.88884000	0.31341100
C	-1.59498400	-0.32554300	0.22460600
C	1.13955600	0.46389100	-0.23861800
C	0.13327700	1.50641500	0.21797700
C	-1.27456200	1.11269100	-0.24255000
O	1.65877800	-1.86572700	-0.11240100
O	-0.53741800	-1.22097800	-0.21486300
O	2.47160600	0.77523400	0.21398100
O	0.58164400	2.73995400	-0.31454500
O	-2.14661900	2.06710700	0.34789700
H	0.67595000	-0.87453400	1.41316800
H	1.24020700	-2.73559800	-0.05969300
H	-1.64605000	-0.34716800	1.32060700
H	1.13759600	0.40519100	-1.33286100
H	2.57072700	1.73826400	0.16997600
H	0.12630500	1.55244500	1.31702000
H	-0.01071000	3.44207700	-0.01729300
H	-1.31635300	1.16540400	-1.33759500
H	-2.93174700	2.19324000	-0.19422400
C	-2.89587600	-0.87955100	-0.34032000
H	-2.82984200	-0.92260400	-1.43554300
H	-3.70904000	-0.20250300	-0.07086500
O	-3.22951000	-2.13571200	0.21349900
H	-2.65021200	-2.80698500	-0.16084100
Na	3.78472800	-1.03824100	-0.02613000

β-SG1′ (-$C_2H_4O_2$)

C	0.93842600	-0.78737700	0.60556700
C	-1.64472300	-0.28343400	0.29836500
C	1.16960500	0.51332000	-0.14468600
C	0.15612700	1.56054100	0.28058700
C	-1.23062400	1.11399000	-0.22360200
O	1.47282400	-1.88226800	0.01235400
O	-0.48302000	-1.19885300	0.38702700
O	2.53887400	0.85725800	0.09835300
O	0.56363300	2.77939300	-0.31153800
O	-2.17827300	2.06316400	0.24744600
H	1.10804300	-0.68721600	1.68537800
H	0.08843200	-2.01264900	-0.20396700
H	-1.99773400	-0.17936600	1.32671100
H	1.04094900	0.31693400	-1.21744400
H	2.64849700	1.80490100	-0.06776100
H	0.12780500	1.65683900	1.37498600
H	0.00088500	3.49493600	0.00879900
H	-1.19720100	1.11274000	-1.31955800
H	-2.77297200	2.33138700	-0.45976700
C	-2.69623100	-0.96447100	-0.57280500
H	-2.29442700	-1.09882800	-1.58200200
H	-3.56079000	-0.29419600	-0.64318800
O	-3.04613200	-2.24745800	-0.10508200
H	-3.74077100	-2.18831300	0.55913300
Na	3.58641500	-1.28567900	-0.32276000

β-SG2

C	-0.32540100	1.71552400	0.32705600
C	1.64452300	0.36369800	0.29484100
C	-1.18229100	0.58012400	-0.24116000
C	-0.60574400	-0.73166900	0.24521800
C	0.84619100	-0.86287800	-0.20147300
O	-0.87418500	2.89566600	-0.15903800
O	1.00066900	1.56804000	-0.14446300
O	-2.55703000	0.67908200	0.18376400

O	-1.40355400	-1.82761200	-0.25161200
O	1.28143600	-2.09632700	0.33823900
H	-0.32967000	1.69308500	1.42907900
H	-0.41239300	3.65786000	0.21131300
H	1.69353000	0.33281800	1.39220500
H	-1.13641300	0.64603300	-1.33346500
H	-2.82003300	1.60696700	0.10238300
H	-0.63290000	-0.76329000	1.34186900
H	-0.85416300	-2.62338400	-0.18388700
H	0.88560300	-0.88245200	-1.30058500
H	2.24236900	-2.15703300	0.21526000
C	3.05691000	0.42187800	-0.28213100
H	3.60268500	1.25038400	0.17829200
H	2.99438900	0.59656400	-1.36206000
O	3.67928600	-0.83384800	0.00282600
H	4.59629900	-0.82368300	-0.28887100
Na	-3.58612800	-1.32126700	-0.09212400

β-SG2 (-H_2O)

C	-0.32154500	1.44312600	0.80023000
C	1.73696800	0.22070600	0.47147300
C	-1.01883500	0.43790900	-0.08432600
C	-0.57128900	-0.92052600	0.48524300
C	0.90241600	-1.04931000	0.10328500
O	-0.88616800	2.82705900	-0.35997700
O	0.95249200	1.35947000	1.01759400
O	-2.34262500	0.74967800	-0.18098300
O	-1.36920600	-1.94693400	-0.11902000
O	1.41347800	-2.20510400	0.74020400
H	-0.87401400	1.87968900	1.62790000
H	-1.04660400	3.67500200	0.07763200
H	2.36780800	-0.04006800	1.32089700
H	-0.51423800	0.51104800	-1.07181000
H	-1.77115900	2.33053600	-0.46675600
H	-0.69296100	-0.97392000	1.57473300
H	-0.96724300	-2.80070700	0.09144000
H	0.94321600	-1.17674200	-0.98381200
H	2.25496200	-2.44427500	0.33116500

C	2.61397600	0.71911100	-0.67115700
H	3.23691300	1.54786900	-0.32076200
H	1.99883500	1.06853200	-1.51010100
O	3.39009500	-0.41818600	-1.03042800
H	4.07138900	-0.17099300	-1.66384200
Na	-3.48378000	-1.03999300	-0.56129800

β-SG2′

C	0.11949100	1.56592400	0.27764500
C	1.63876600	-0.27711000	0.23182700
C	-1.03415900	0.70306900	-0.24053400
C	-0.82037000	-0.71894100	0.23509900
C	0.53106500	-1.23702600	-0.25289200
O	-0.10835400	2.84650700	-0.21209400
O	1.33054600	1.04942700	-0.23785600
O	-2.31318400	1.17014900	0.23300400
O	-1.90557200	-1.54599000	-0.23403800
O	0.62305900	-2.55171900	0.28637800
H	0.15273000	1.55573200	1.37894000
H	0.53448600	3.46618000	0.15394500
H	1.67288700	-0.28395300	1.32984200
H	-1.01501700	0.75227300	-1.33477300
H	-2.31369200	2.13540500	0.15844300
H	-0.82177300	-0.74612300	1.33235100
H	-1.61009700	-2.46507300	-0.15097200
H	0.53338900	-1.26688300	-1.35025700
H	1.30334200	-3.06147500	-0.16634300
C	3.02503900	-0.61591400	-0.30531700
H	3.00961000	-0.56816500	-1.40270100
H	3.28848900	-1.63357800	-0.00692500
O	4.02105200	0.22080300	0.23974400
H	3.90001300	1.11156600	-0.10668000
Na	-3.87034000	-0.45721200	-0.01008600

β-SG2′ (-H_2O)

C	-0.15384700	-1.17536300	0.90708500

C	-1.69351300	0.55467100	0.23132700
C	0.84416700	-0.56920100	-0.05035300
C	0.86787200	0.90914600	0.36984800
C	-0.47928300	1.49660200	-0.06585000
O	-0.05108600	-2.80234200	-0.02877000
O	-1.33161400	-0.65234000	1.03845900
O	1.98876900	-1.31124500	-0.04954300
O	1.97349100	1.54650800	-0.28320500
O	-0.59735000	2.75199600	0.58584800
H	0.21994500	-1.63493900	1.81849200
H	-0.16158600	-3.58666500	0.52727800
H	-2.36368800	1.06586200	0.92140900
H	0.36023700	-0.57852600	-1.04962500
H	0.95021500	-2.62042300	-0.15866100
H	0.98371800	1.02477200	1.45484900
H	1.92954500	2.49383400	-0.09706700
H	-0.42358500	1.63821700	-1.15279500
H	-1.23900600	3.31512000	0.13829900
C	-2.48846500	0.12258900	-0.99992700
H	-1.88408100	-0.52369900	-1.64905700
H	-2.72931600	1.02575700	-1.56869900
O	-3.71928600	-0.47091700	-0.66066100
H	-3.58206400	-1.37733900	-0.36669800
Na	3.67769800	-0.06962800	-0.54432100

β-SG1

C	-0.16423600	1.38184800	0.51530400
C	0.51042100	0.94618100	-0.81347700
C	-0.79736100	-1.15614700	-0.95631600
C	-1.78696800	-0.50117100	0.03672500
C	-1.01653900	0.25310700	1.12976400
H	-0.00375400	1.45869100	-1.63333400
H	-1.25191300	-1.17911300	-1.95033400
H	-2.36762000	-1.31428800	0.48043700
H	-1.72317200	0.70198300	1.83295000
H	0.59105800	1.67315700	1.24979700
O	0.46264400	-0.47560300	-1.01098500
O	-0.44381400	-2.45890900	-0.52356800

H	-0.55593100	-3.08827300	-1.24408600
O	-2.69459200	0.34092600	-0.64631200
H	-2.42255300	1.26789100	-0.57906700
O	-0.12458800	-0.63414600	1.83936800
H	-0.61499700	-1.08106400	2.53828200
O	-0.99558300	2.49352900	0.16959800
H	-1.15688800	3.05097800	0.93967100
C	1.98772100	1.29611000	-0.87400800
H	2.38577900	1.05611000	-1.86319000
H	2.11438100	2.36507000	-0.68162400
O	2.66960200	0.51375100	0.13271000
H	3.55799400	0.86310100	0.25868500
Na	1.64182100	-1.57547200	0.61248800

β-SG1 (-H_2O)

C	0.78838900	-1.00473600	0.80764500
C	0.28022300	-1.32903100	-0.61166100
C	0.59856600	0.99967800	-1.27181700
C	1.43318700	1.26638400	-0.04398100
C	0.78931300	0.51034000	1.13858600
H	1.07286900	-1.88197000	-1.12028600
H	0.50947300	1.70354400	-2.09417000
H	1.45450500	2.33698500	0.15854100
H	1.44832700	0.64000300	2.01453000
H	0.14860700	-1.50595000	1.53827000
O	0.11509700	-0.13891100	-1.52144100
O	-1.40974500	2.29289100	-0.50323600
H	-1.47367000	3.25260900	-0.56399600
O	2.73279900	0.86435200	-0.46445700
H	2.91175900	-0.02868800	-0.12048100
O	-0.48490200	0.97353300	1.33479500
H	-0.92570000	2.00269400	0.36798900
O	2.12010100	-1.55280500	0.83578600
H	2.41199000	-1.66056100	1.74910500
C	-0.97826900	-2.15504600	-0.76510800
H	-1.19183300	-2.28218600	-1.83034500
H	-0.75862200	-3.13644500	-0.33176400
O	-2.11206400	-1.56750600	-0.10527000

H	-2.83470900	-2.20460300	-0.15302700
Na	-2.53925000	0.55150900	0.75038500

β-SG4

C	-0.16355600	1.38157500	0.51565900
C	0.51090300	0.94587500	-0.81320600
C	-0.79759000	-1.15580300	-0.95662100
C	-1.78722700	-0.50031700	0.03595800
C	-1.01674500	0.25310600	1.12959100
H	-0.00340900	1.45819200	-1.63307900
H	-1.25123900	-1.17820300	-1.95105500
H	-2.36875800	-1.31315500	0.47904500
H	-1.72335700	0.70235200	1.83255300
H	0.59177700	1.67215500	1.25039800
O	0.46297300	-0.47597100	-1.01030100
O	-0.44514300	-2.45885100	-0.52383600
H	-0.55660000	-3.08791200	-1.24471900
O	-2.69389000	0.34285000	-0.64705200
H	-2.42150500	1.26966500	-0.57892800
O	-0.12566800	-0.63473400	1.83945700
H	-0.61661500	-1.08140000	2.53816000
O	-0.99421600	2.49391600	0.17023000
H	-1.15450100	3.05179200	0.94020300
C	1.98823800	1.29566800	-0.87391700
H	2.38613100	1.05627200	-1.86331200
H	2.11512400	2.36448300	-0.68085000
O	2.67000000	0.51252300	0.13226400
H	3.55868800	0.86120400	0.25802200
Na	1.64069700	-1.57581400	0.61297000

β-SG4 (-H_2O)

C	0.76541200	1.00991300	-0.81538000
C	0.29590800	1.30418000	0.63748000
C	0.56161200	-1.04954900	1.25494800
C	1.45527000	-1.25224200	0.05069000
C	0.81453100	-0.50681000	-1.13505000
H	1.11543200	1.79314400	1.16581700
H	0.41695100	-1.79163000	2.03530800

H	1.55557800	-2.31539700	-0.16821700
H	1.47777200	-0.61990200	-2.00645300
H	0.03201700	1.43419900	-1.50187800
O	0.07005800	0.07575200	1.51522800
O	-1.43519100	-2.35141400	0.44502200
H	-1.53825400	-3.30946400	0.45692800
O	2.70005000	-0.66072100	0.45457200
H	3.35424300	-1.33569600	0.67020900
O	-0.45117700	-1.00960400	-1.32670100
H	-0.92450100	-2.03298100	-0.40834500
O	1.96997400	1.70917600	-1.05677500
H	2.70813600	1.20412700	-0.69113200
C	-0.93635700	2.15829700	0.82420600
H	-1.15016700	2.27220200	1.89082700
H	-0.69588700	3.14035300	0.40403900
O	-2.08015200	1.59740300	0.15359300
H	-2.78484600	2.25507500	0.18098100
Na	-2.49938400	-0.50559000	-0.76445000